

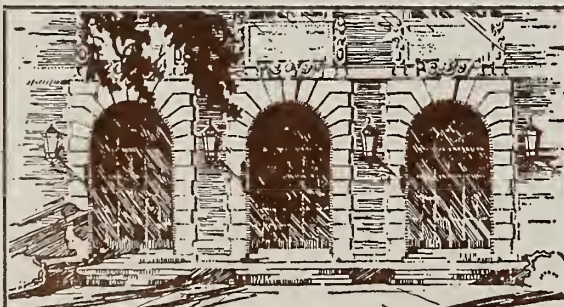
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THE ENERGY TRANSPORT PROPERTIES
OF ONE DIMENSIONAL ANHARMONIC LATTICES

By

KEN'ICHI MIURA

July 20, 1973

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July 20, 1973

Department of Computer Science
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801

*Submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Computer Science in the Graduate College of the University of Illinois at Urbana-Champaign and supported in part by the Department of Computer Science and the Advanced Research Projects Agency of the Department of Defense and was monitored by the U.S. Army Research Office-Durham under Contract No. DAHCO-4-72-C-0001.

THE ENERGY TRANSPORT PROPERTIES
OF ONE DIMENSIONAL ANHARMONIC LATTICES

BY

KEN'ICHI MIURA

B.S., University of Tokyo, 1968
M.S., University of Illinois, 1971

THESIS

Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Computer Science
in the Graduate College of the
University of Illinois at Urbana-Champaign, 1973

Urbana, Illinois

THE ENERGY TRANSPORT PROPERTIES
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Ken'ichi Miura, Ph.D.
Department of Computer Science
University of Illinois at Urbana-Champaign, 1973

The energy transport properties of the solitary waves are studied both analytically and numerically. It was found that the piecewise linear function model clearly explains the characteristics of such waves. Numerical experiments were performed extensively to clarify the various properties of the solitary waves in the one dimensional anharmonic lattice. These results were used to interpret the heat conduction problem of the crystal lattice.

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CHAPTER 1. INTRODUCTION

1.1 Historical Introduction

The heuristic approach to solve mathematical problems in physics has attracted attention of physicists since the advent of digital computers. Undoubtedly, J. von Neumann was the first to propose such approach. In 1944 he solved a simple hydrodynamical problem numerically by using the then available punch-card equipment at the Ballistic Research Laboratory which was developed by IBM for calculating firing and bombing tables.⁽¹⁾ (Note that the first electronic computer ENIAC was yet to be completed at that time!) He solved the one dimensional hydrodynamical equation for shock waves in Lagrangian coordinates:

$$x_{tt} = F'(x_a)x_{aa}$$

where $x(a,t)$ is the position of a moving fluid particle with Lagrangian coordinate a at time t , and $F(x_a)$ gives the pressure vs specific volume relation (homotropic equation of state). His idea was to discretize the spatial coordinate a in order to reduce the above partial differential equation to a set of ordinary differential equations of the form:

$$m \frac{d^2 x_n}{dt^2} = f(x_{n+1} - x_n) - f(x_n - x_{n-1}). \quad (1.1)$$

This is nothing but the equation of motion for an array of identical-mass particles connected by springs. (Fig. 1.1) He observed a shock wave formed in such mechanical system for $f(x) = (1 - \frac{x}{2})^2$, $0 < x \leq 2$.^{*} This was the first numerical experiment ever made on a computing device. He further discussed that the extensive but well planned computational efforts would break the deadlock encountered by purely analytical approach

* Since there is no dissipative term in (1.1), the shock wave which von Neumann observed is essentially a solitary wave which is to be described in the next section. One of Von Neumann's results is reproduced in Fig. 1.2.



Fig. 1.1. Mass-spring system.

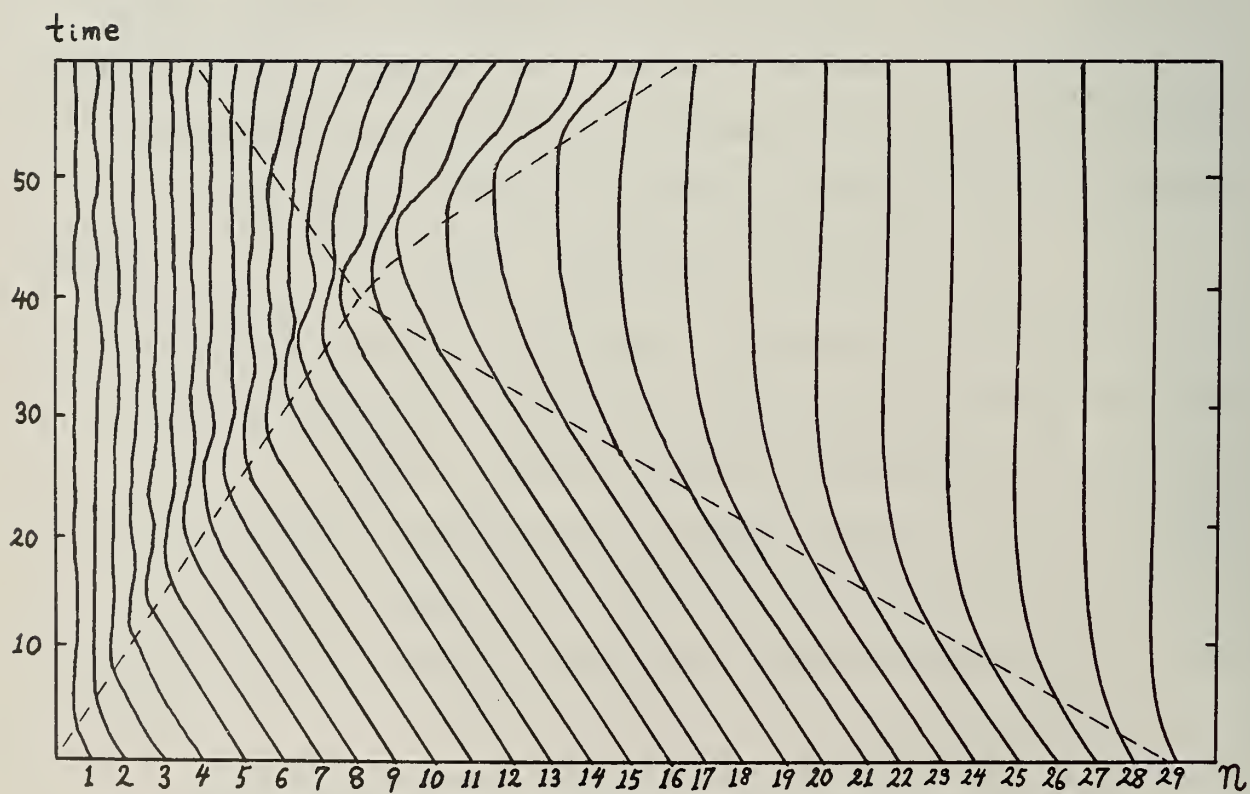


Fig. 1.2. Shock wave in the system (1.1).

in such problems as turbulence and shock waves.⁽²⁾ The next great step was made by Fermi, Pasta and Ulam, who studied the behavior of the vibration in a nonlinear string on MANIAC I computer at Los Alamos scientific laboratory in 1953.⁽³⁾ Their model was also a discrete one; the equation of motion is identical to (1.1) with the function f given as:

$$(1) \quad f(x) = x + \alpha x^2 \quad (\text{quadratic nonlinearity})$$

$$(2) \quad f(x) = x + \beta x^3 \quad (\text{cubic nonlinearity})$$

$$(3) \quad f(x) = \begin{cases} \delta_1 x & |x| \leq d \\ \delta_2 x + c & |x| > d \end{cases} \quad (\text{broken linear function})$$

where α , β , δ_1 , δ_2 , c and d are given parameters. Their intention was to observe the mixing of energy among the normal modes of the system due to a weak nonlinearity. The result was, however, quite contrary to what they expected: starting with the initial energy given to the lowest mode, only a few modes were excited, after which almost all the energy was returned to the original mode. This result cast doubt on the long-believed hypothesis that only a slight nonlinearity will lead a dynamical system to a statistically equilibrium state. This numerical experiment by Fermi, Pasta and Ulam will be referred to as FPU throughout this paper.

The FPU experiment has stimulated extensive research during the last two decades, both computationally and analytically, among physicists and mathematicians. The research directions may be categorized into several areas:

- (1) ergodic (or non-ergodic) behavior of nonlinear vibrating systems,
- (2) theory of the normal mode coupling,
- (3) thermal conductivity in the anharmonic crystals

(4) energy transport properties of nonlinear vibrating systems (especially in relation to the continuum approximation).

Of course these areas are not independent of each other, but closely related. Here, particular attention should be paid to the last area because a special type of solution has been discovered in such dynamical systems: that is, the solitary wave (or the "soliton" as was named by Zabusky and Kruskal⁽⁴⁾). As a matter of fact the solitary wave has been known in hydrodynamics since 1844, when Scott Russel reported a single elevation of water in a long canal which propagated without changing its shape.⁽⁵⁾ Theoretical investigations that followed by Lord Rayleigh,⁽⁶⁾ Boussinesq,⁽⁷⁾ Kortweg and deVries⁽⁸⁾ clarified the nature of such wave; especially Kortweg and deVries derived the equation which is now known as KdV equation:

$$u_t + uu_x + Bu_{xxx} = 0 \quad (1.2)$$

where u is the velocity of the water. The maintenance of the wave is possible due to the balancing of two different effects: the nonlinearity that tends to sharpen the wave front, and the dispersion that tends to spread out the wave front. Recently the solitary waves have been discovered in plasma waves and ion-acoustic waves as well as in the anharmonic crystals, and much effort has been concentrated on the analysis of such waves. As for the crystal lattices, Zabusky and Kruskal showed that the equation of motion (1.1) may be reduced to KdV equation or its variations by introducing new coordinates,⁽⁹⁾ and using an appropriate approximation. Toda^{(10), (11)} found a particular solution of the solitary wave type for the so called "exponential lattice", which is described by a force function $f(x) = (1 - \exp(-bx))/b$. This is the only exact solution known for any anharmonic lattice.

As for the ergodic problems, many numerical experiments have been done under various conditions. The original FPU situation was re-examined by Tuck for longer periods of time, resulting in the "super recurrence".⁽¹²⁾ On the other hand, the system approached to the thermal equilibrium for a strong nonlinearity⁽¹³⁾ or for an initial condition given to the higher mode.⁽¹⁴⁾ The phenomenon of FPU recurrence was studied from the viewpoint of the normal mode coupling by Ford,^{(15),(16)} Jackson⁽¹⁷⁾ and Pasta et al.⁽¹⁸⁾ Jackson could quantitatively show the behavior of a few lower modes, which is quite in good agreement with the result obtained by FPU.

The development of the area of the heat conduction will be discussed more in detail in the next section.

1.2 Problems of Heat Conduction

Among several published reports on numerical experiments of the heat conduction problem,^{(19),(20)} the one by Jackson, Pasta and Waters⁽²¹⁾ (to be referred to as JPW throughout this thesis) is very well documented on the computational aspects of their model too. Therefore we will describe the problem along the lines of their report.

Let us consider a one dimensional lattice which consists of N atoms of identical mass m connected by anharmonic springs. We choose free boundary conditions on both ends. The force function is of polynomial type:

$$f(x) = x - \lambda x^2 + \mu x^3 \quad (1.3)$$

where λ and μ are the nonlinear coefficients for the quadratic and cubic terms, respectively. The special relation $\mu = 2\lambda^2/3$ or $\mu = \frac{\lambda^2}{4}$ is used to assure that the force is always attractive. λ may be varied from one spring to another (JPW called this "defects"), but we will only be concerned

with a constant λ in all cases. Next we define a heat reservoir in the following way; every time an end particle hits the reservoir, it loses its velocity and is kicked back toward the lattice with a new velocity v sampled from the probability density function

$$p(v) = (v/T)\exp(-v^2/2T). \quad (1.4)$$

This definition was given by JPW and is very well suited for numerical experiments on digital computers. The lattice is located between two heat reservoirs of given temperatures and is subject to random motion. If two temperatures are different we expect an energy flow from the high temperature side to the low temperature side. In other words we can define the heat flux $\bar{J}$ numerically by the time-averaged energy transferred through the lattice. We can also define the temperature of each atom, either by time-averaged kinetic energy or by time-averaged total energy. Usually the former is chosen for its simplicity. Fourier's law of heat conduction states that the heat flux J is proportional to local temperature gradient so that the thermal conductivity can be defined as follows:

$$J = -\kappa \nabla T.$$

Computationally, κ can be calculated from the averaged heat flux $\bar{J}$ and the linear-interpolated temperature distribution. JPW performed several types of numerical experiments on the lattice-reservoir system just described. As they mentioned in the general description of their results, pulse-like waves are observed to propagate through the lattice without much distortion in spite of the irregular motions of atoms and defects (Fig. 2 and Fig. 3 of (21)). This fact suggests that the phenomenon of heat conduction might be considered in terms of localized waves (such as those we introduced in

§1.1). This leads to such questions as:

- (1) Is it possible to create solitary waves by impulse type initial conditions?
- (2) If so, do such waves propagate through the lattice without appreciable dispersion of energy?
- (3) How do such waves contribute to energy transfer?
- (4) What are the effects of boundaries?
- (5) What will be the possible sources of the temperature gradient for anharmonic lattices which was observed by JPW and other authors?

And so on.

Our main purpose in this thesis is to establish a dynamical picture of the heat conduction through the lattice in terms of the localized waves and also to find the limitation of such approach. We will also discuss some of the related topics herein.

1.3 Outline of This Thesis

This thesis consists of two parts, one being on the mathematical derivations and the other being on the numerical experiments. In Chapter 2 we will study the dynamical properties of the harmonic lattices. An emphasis will be put on the solutions discovered by Schrödinger, which are very convenient for describing localized solutions. Some of the thermal properties of the harmonic lattice will be also described. In Chapter 3 we will discuss the properties of the anharmonic lattices; first in continuum approximation and then about Toda's exponential lattice. The solitary wave solutions and the periodic wave solutions are obtained in both cases. The special features of such solutions will be extensively discussed and they will be simply explained in terms of elementary functions. Chapter 4 is about the numerical methods and some related problems encountered in

the actual computation. We will show that Nyström's integration formula for the special equations of the second order is quite advantageous for our purpose. In Chapter 5 we will analyse the computational results on the basic dynamical properties of our model lattice. Specifically we will show that the solitary waves can be created when the lattice interacts with the heat reservoirs. Since no exact solution is known for our model lattice, the results obtained in Chapter 3 are applied whenever applicable. In Chapter 6 we will discuss the heat conduction problem, considering the results in Chapter 5, our own computational results in the thermal situation as well as those obtained by JPW and other authors. Some of the questions raised in §1.2 will be answered.

CHAPTER 2. THE HARMONIC CRYSTAL LATTICES

We consider the one dimensional crystal lattices in this chapter which consist of either an infinite or finite number of atoms of identical mass and connecting springs which obey Hook's law, $f(x) = Kx$. The equation of motion for the displacement y_n of the n^{th} atom from its equilibrium position is then

$$m \frac{d^2 y_n}{dt^2} = K(y_{n+1} - 2y_n + y_{n-1}) \quad (2.1)$$

Boundary conditions and initial conditions are to be described later.

The linear theory of lattice vibration has a very long history in the theoretical physics, or we should rather say that a considerable part of mathematical physics was developed around this very subject in its early stages. Newton was the first to investigate this problem. He speculated that "the phenomena of Nature....may all depend on certain forces by which the particles of bodies...are either mutually impelled towards one another, and cohere in regular figures or are repelled..." (Principia). It is along this line that Newton considered how the sound wave propagates in the air. By discretizing the continuous media such as air into particles of mass m he obtained the equation of motion identical to (2.1). Note that the theory of the partial differential equations was not developed at this time. Newton's idea was developed by Bernoulli, Lagrange, Cauchy, Hamilton and many other well known mathematical-physicists. For more details on the historical development of the theory, we refer the reader to L. Brillouin.⁽²²⁾ The basic idea behind the development of the theory of harmonic lattices is the decomposition of the vibratory motion into the Fourier components, or the normal modes of the system.

2.1 Normal Mode Representation of the Vibration of the Harmonic Lattices

Suppose that we have a finite number of atoms. The normal mode representation is obtained by putting the solution of (2.1) in the following form:

$$y_n(t) = f_n \exp(i\omega t).$$

Substituting (2.2) into (2.1) yields a finite difference equation for f_n :

$$f_{n+1} - (2 - \frac{m}{K}\omega^2)f_n + f_{n-1} = 0,$$

which we can solve by putting $f_n = \exp(ikn)$. By defining $\omega_0 = 2\sqrt{\frac{K}{M}}$, we obtain the dispersion relation

$$\omega = \omega_0 \sin(k/2) \quad 0 \leq k \leq \pi. \quad (2.2)$$

The system is dispersive for large k . The values of possible k 's depend on the boundary condition, but in general there are N distinct k 's (we call them the modes of the system) if there are N atoms in the system. The larger the number of atoms in the system, the greater the density of the allowed values along the k axis. Note that ω is always less than ω_0 . This is why the mass-spring system is often called the mechanical low-pass filter. Actually we can show that there is a close correspondence between the mechanical filters and the electrical filters (section 2.3). Also refer to L. Brillouin. (22)

Going back to the problem of finding the k 's for a given boundary condition, we take the following steps⁽²³⁾:

- (i) Put $f_n = A \exp(ikn) + B \exp(-ikn)$ and find k 's that satisfy the boundary condition.
- (ii) Express B (or A) in terms of A (or B) to obtain a unique representation for f_n . This gives a set of orthogonal functions from

which we can obtain a set of orthonormal functions.

- (iii) Obtain ω for each k . They are all located on the sine curve given in (2.2).

Some typical boundary conditions are listed in Table 2.1 together with the values of k and ω , and normal coordinates.

There is another type of solution for an infinite lattice which is obtained by putting

$$y_n(t) = f_n \cdot \exp(-2\beta t) \quad (2.3)$$

where

$$f_n = \exp(2\alpha n). \quad (2.4)$$

Following the same procedures as before, we can obtain the relation between α and β as:

$$\beta = \omega_0 \sinh(\alpha). \quad (2.5)$$

Because of its unboundedness this solution is seldom mentioned. If the amplitude growth is suppressed by some nonlinear effect, however, the resulting solution will have an exponential behavior in the region in which the amplitude is sufficiently small. This is actually the case for Toda's solitary wave solution. We will come back to this problem in §3.5.

Going back to the normal mode representation, we can find the solution of (2.1) for a given initial condition by superposing the normal modes. As an example, let us consider the wave motion when the left end atom of a free-ended lattice is given an impulse of unit magnitude at $t=0$. The general solution is:

$$y_n(t) = A_0 + B_0 t + \sum_{m=1}^{N-1} \left[A_m \cos(\omega_m t) + \frac{B_m}{\omega_m} \sin(\omega_m t) \right] \cos[m\pi(2n+1)/2N] \quad (2.6)$$

Table 2.1

Normal Mode Representation

periodic

$$y_n^m(t) = a_m(t) \exp(2\pi i m n / N) \quad m = 1, 2, \dots, N$$

$$\text{where } a_m(t) = \exp(i\omega_m t)$$

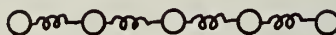
$$\text{and } \omega_m^2 = \frac{K}{m} \sin^2(\pi m / 2N)$$

free ends

$$y_n^m(t) = a_m(t) \cos[\pi m (2n+1) / 2N] \quad m = 0, 1, \dots, N-1$$

$$\text{where } a_m(t) = \exp(i\omega_m t)$$

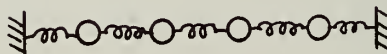
$$\text{and } \omega_m^2 = \frac{K}{m} \sin^2(\pi m / 2N)$$

fixed ends

$$y_n^m(t) = a_m(t) \sin(\pi m n / N) \quad m = 1, 2, \dots, N-1$$

$$\text{where } a_m(t) = \exp(i\omega_m t)$$

$$\text{and } \omega_m^2 = \frac{K}{m} \sin^2(\pi m / 2N)$$



where A_m and B_m are the Fourier coefficients of the initial displacement and velocity which will be given shortly. We can also obtain $\dot{y}_n(t)$ as follows:

$$\dot{y}_n(t) = B_0 + \sum_{m=1}^{N-1} [B_m \cos(\omega_m t) - A_m \omega_m \sin(\omega_m t)] \cos[m\pi(2n+1)/2N]. \quad (2.7)$$

Initial conditions are

$$y_n(0) = A_0 + \sum_{m=1}^{N-1} A_m \cos[m\pi(2n+1)/2N] \quad (2.8)$$

and

$$\dot{y}_n(0) = B_0 + \sum_{m=1}^{N-1} B_m \cos[m\pi(2n+1)/2N]. \quad (2.9)$$

Or solving for A_m and B_m ,

$$A_m = \frac{\epsilon_m}{N} \sum_{n=0}^{N-1} y_n(0) \cos[m\pi(2n+1)/2N] \quad (2.10)$$

$$B_m = \frac{\epsilon_m}{N} \sum_{n=0}^{N-1} \dot{y}_n(0) \cos[m\pi(2n+1)/2N] \quad (2.11)$$

where $\epsilon_m = \begin{cases} 1 & \text{if } m=0 \\ 2 & \text{if } m \neq 0 \end{cases}$. A_0 and B_0 give the motion of the center of mass of the lattice. For the present problem, we have the following initial conditions:

$$y_n = 0 \text{ for all } n \implies A_m = 0 \text{ for all } m,$$

$$\dot{y}_n = \delta_{n,0} \implies B_m = \frac{\epsilon_m}{N} \cos(m\pi/2N).$$

Substituting A_m and B_m into (2.7) yields

$$\dot{y}_n(t) = 1/N + \frac{2}{N} \sum_{m=1}^{N-1} \cos(m\pi/2N) \cos[t \sin(m\pi/2N)] \cos[m(2n+1)\pi/2N]. \quad (2.12)$$

This is the solution for the given initial condition. Note that the amplitude distribution among the normal modes is not uniform but shows a monotonous decrease as the mode number increases. The energy distribution is obtained from the square of the amplitude distribution, since initially there is no potential energy and the total energy of each mode is strictly conserved. Both distributions are shown in Fig. 2.1 and Fig. 2.2. For the anharmonic lattices with the same boundary and initial condition we can also use this distribution approximately if time is very close to $t=0$. This will be discussed in §5.1.

Next let us consider the case when N goes to infinity. From (2.12) we have

$$\dot{y}_n(t) = \frac{4}{\pi} \int_0^{\pi/2} \cos(x) \cos[t \sin(x)] \cos[(2n+1)x] dx + O(1/N) \quad (N \rightarrow \infty)$$

where

$$\begin{aligned} x &= \frac{m\pi}{2N}, \quad dx = \frac{\pi}{2N}, \\ &= \frac{4}{\pi} \int_0^1 \cos(wt) \cos[(2n+1)\arcsin(w)] dw \end{aligned}$$

where

$$\begin{aligned} w &= \sin x, \quad dw = \cos x \, dx, \\ &= \frac{4}{\pi} \int_0^1 \cos(wt) (-1)^n U_{2n+1}(w) dw, \end{aligned} \quad (2.13)^*$$

where $U_{2n+1}(w)$ is the second kind of solutions of Tchebycheff's equation: $(1-w^2)d^2U_n(w)/dw^2 - w dU_n(w)/dw + n^2 U_n(w) = 0$. Making use of the following identity for an odd n ,

$$\frac{2}{\pi} \int_0^1 (-i)^{n-1} \frac{U_n(w)}{n} \cos(wt) dw = \frac{J_n(t)}{t}, \quad (A.7)^*$$

* See Appendix A for the derivation.

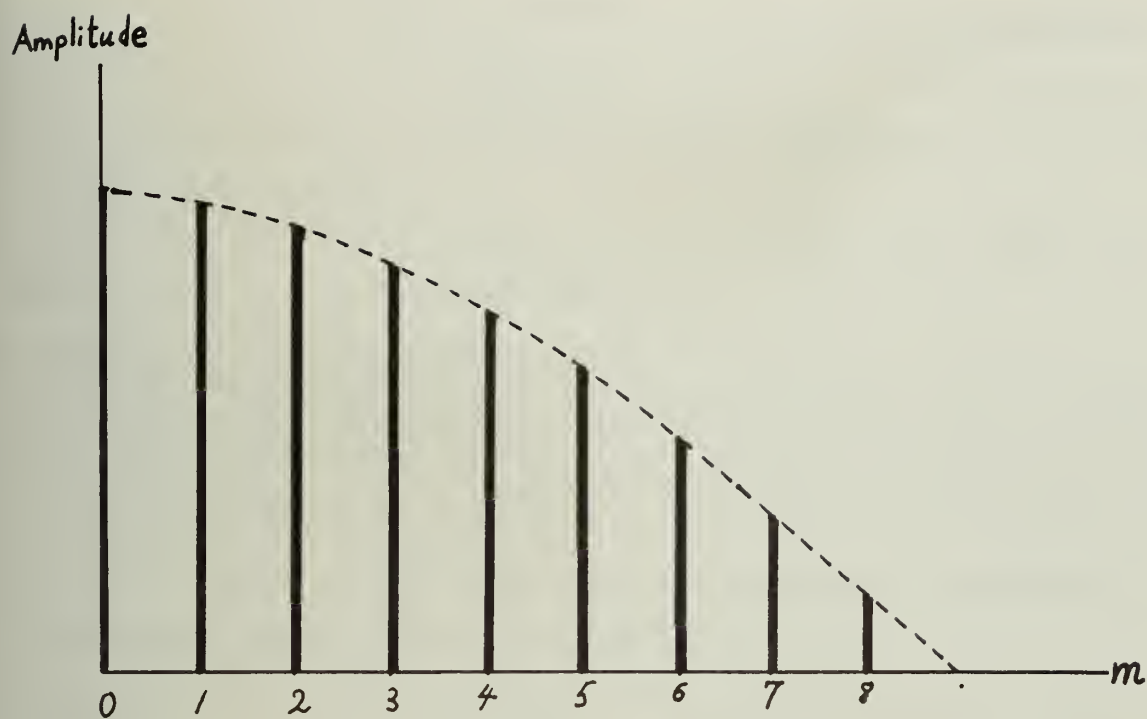


Fig. 2.1. Amplitude distribution ($N=9$).

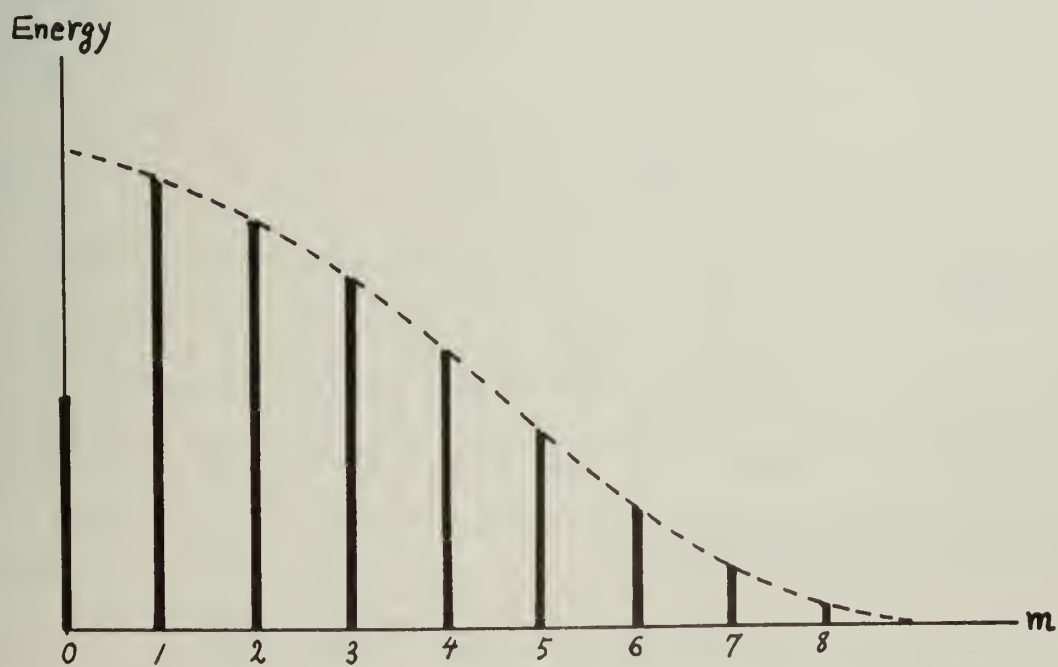


Fig. 2.2. Energy distribution ($N=9$).

we can obtain the expression for $\dot{y}_n(t)$ when $N \rightarrow \infty$:

$$\dot{y}_n(t) = 2(2n+1) \frac{J_{2n+1}(t)}{t} . \quad (2.14)$$

We will obtain this solution much more easily in the next section. This solution is the response of the velocity of the n^{th} atom to a unit impulse at the left end; it shows how the energy propagates through the harmonic lattice. In a thermal situation initial impulses are given at random. We will come back to this problem in §2.4.

2.2 Schrödinger's Solutions

A different type of solutions was found by Schrödinger in 1914 for infinite harmonic lattices.⁽²⁴⁾ Since his solutions are very convenient for describing the energy transport through the lattice we will summarize some of their features.

Let us introduce the new coordinates η_n according to Schrödinger;

$$\eta_{2n} = \sqrt{m} \dot{y}_n \quad (2.15a)$$

$$\eta_{2n+1} = \sqrt{K}(y_n - y_{n+1}) \quad (2.15b)$$

and $t' = \omega_0 t$, where $\omega_0^2 = 4K/m$. Then (2.1) yields

$$d\eta_{2n}/dt' = (\eta_{2n-1} - \eta_{2n+1})/2 \quad (2.16a)$$

$$d\eta_{2n+1}/dt' = (\eta_{2n} - \eta_{2n+2})/2 . \quad (2.16b)$$

These equations are equivalent to

$$d\eta_n/dt' = (\eta_{n-1} - \eta_{n+1})/2 \quad (2.17)$$

which is a recurrence formula for Bessel functions and Neumann functions.⁽²⁵⁾

Since Bessel functions with integer order are the only ones which are finite for all $t' \geq 0$, we will restrict ourselves to such solutions. Therefore the general solution is given as a linear combination of Bessel functions as follows:

$$\eta_n = \sum_k a_k J_{n-k}(t') , \quad (2.18)$$

where a_k 's are determined from the initial conditions. Let us consider an initial impulse given to the 0^{th} atom when all the atoms are in their equilibrium positions. Eventually we will consider the example discussed in §2.1 in terms of Schrödinger's solutions. We have, for the present example, $a_k = \sqrt{m} \delta_{k,0}$, or

$$\eta_n = \sqrt{m} J_n(t') .$$

Going back to the original coordinates, we have

$$\dot{y}_n = J_{2n}(\omega_0 t) \quad (2.19)$$

$$\begin{aligned} y_n - y_{n+1} &= \sqrt{m/K} J_{2n+1}(\omega_0 t) \\ &= \frac{2}{\omega_0} J_{2n+1}(\omega_0 t) . \end{aligned} \quad (2.20)$$

In general Schrödinger's solutions are very convenient for studying the propagation of local disturbances through the lattices. Fig. 2.3 shows how an initially localized disturbance propagates with time. As is clear from Fig. 2.3, the harmonic lattice is very dispersive and energy spreads out rather quickly. From the asymptotic formula for Bessel functions, the amplitude of the wave is known to decay as $(\omega_0 t)^{-1/2}$.⁽²⁵⁾

In order to satisfy the free boundary condition at the left end of the lattice, we add another impulse of the same magnitude to the atom

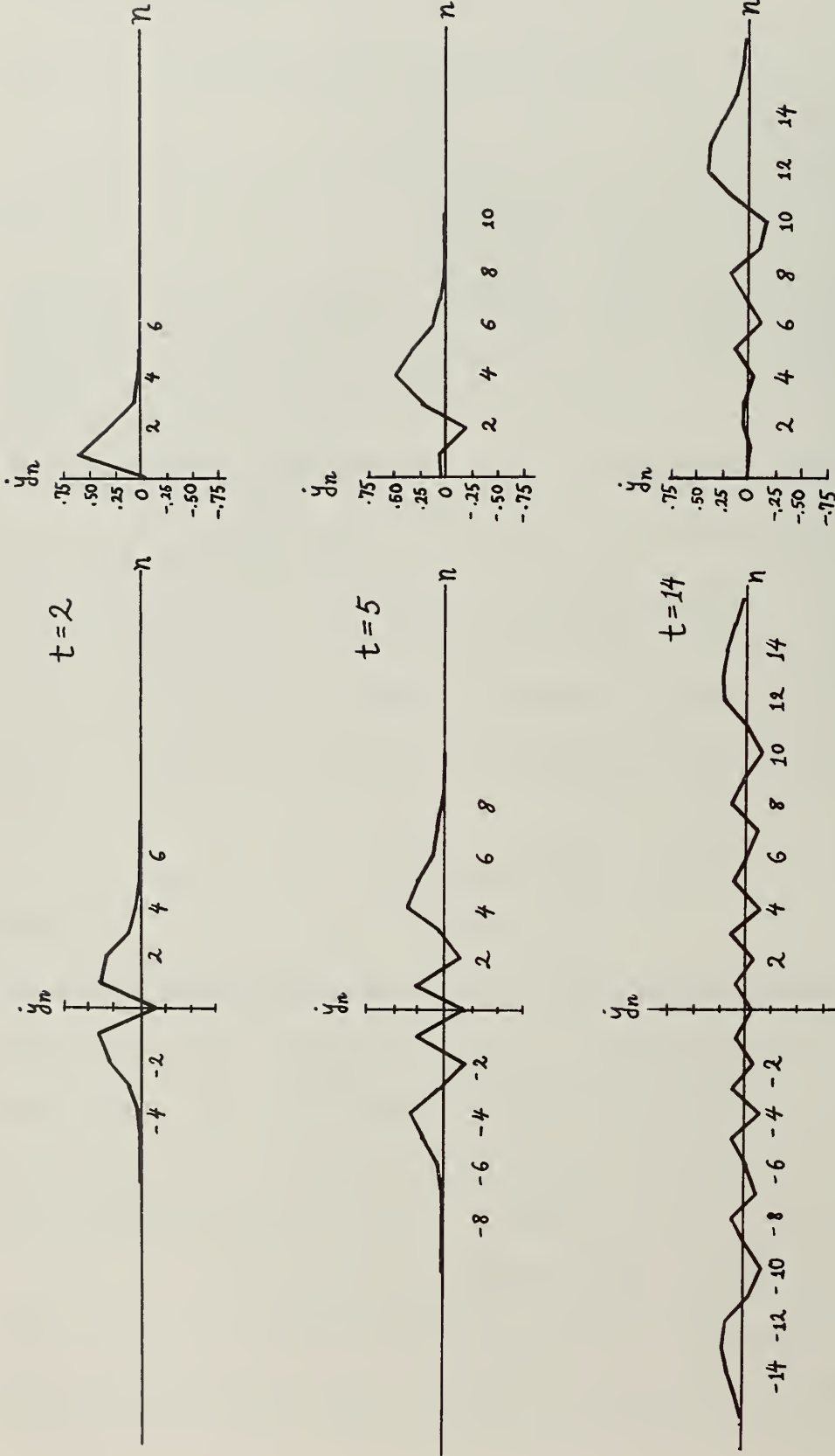


Fig. 2.3a. Schrödinger's solution.

Fig. 2.3b. Semi-infinite Harmonic Lattice.

on the left of atom $n=0$. Then the solution is

$$\dot{y}_n = J_{2n}(\omega_o t) + J_{2n+2}(\omega_o t) . \quad (2.21)$$

In particular the atom $n=0$ and $n=-1$ oscillate exactly in the same way. Initially there is no energy stored in the spring that connects them; therefore atom $n=0$ actually feels no forces from its left neighbor. Consequently we can eliminate all the atoms with negative indices, and the resulting lattice is semi-infinite. By making use of a recurrence formula

$$(J_{n-1} + J_{n+1})/2 = n J_n / x, \quad (2.22)$$

(2.21) may be written as

$$\dot{y}_n = 2(2n+1) J_{2n+1}(\omega_o t) / \omega_o t . \quad (2.23)$$

We can also obtain the response of $y_n - y_{n+1}$ to a unit impulse in the same way:

$$\begin{aligned} y_n - y_{n+1} &= 2/\omega_o [J_{2n+1}(\omega_o t) + J_{2n+3}(\omega_o t)] \\ &= 8(n+1)/\omega_o [J_{2n+2}(\omega_o t) / \omega_o t] . \end{aligned} \quad (2.24)$$

Fig. 2.3 shows how each atom responds to an impulse; we can see that each wave decays somewhat faster than in the previous example. This is due to the fact that there is no force to pull atom $n=0$ back to the original position. (2.24) asymptotically behaves as $(\omega_o t)^{-3/2}$. In the similar way we can obtain the velocity response function when the initial impulse is applied to the k^{th} atom. The results are

$$\dot{y}_n(t) = J_{2(k-n)}(\omega_o t) + J_{2(n+k)+2}(\omega_o t) \quad 0 \leq n < \kappa$$

$$\dot{y}_k(t) = J_0(\omega_0 t) + J_{4k+2}(\omega_0 t) \quad n = k$$

$$\dot{y}_n(t) = J_{2(n-k)}(\omega_0 t) + J_{2(n+k)+2}(\omega_0 t) \quad n > k.$$

It is easy to see that the free boundary condition is satisfied at $n=0$.

Parenthetically, the solution we just obtained is also a solution to the infinitely long lattice with atom $n=0$ twice as heavy as the other atoms, to which an impulse is applied.

Schrödinger's solutions are very simple and clear as long as the lattice is infinite, but in the case of a finite lattice the reflection of waves must be taken into account. Consequently we have an infinite series of Bessel functions instead of a single term, even for the response function to an impulse. For example, the velocity impulse function for a lattice with N atoms ($n=0$ and $n=N-1$ being free ends) is:

$$\begin{aligned} F_n(\omega_0 t) = & J_{2n}(\omega_0 t) + J_{2n+2}(\omega_0 t) + J_{4N-2-2n}(\omega_0 t) + J_{4N-2n}(\omega_0 t) \\ & + J_{4N+4+2n}(\omega_0 t) + J_{4N+2+2n}(\omega_0 t) + J_{8N-2-2n}(\omega_0 t) \\ & + J_{8N-2n}(\omega_0 t) \\ & + \dots \\ = & \sum_{k=0}^{\infty} [J_{4kN+2n}(\omega_0 t) + J_{4kN+2n+2}(\omega_0 t) + J_{4(k+1)N-2n}(\omega_0 t) \\ & + J_{4(k+1)-2}(\omega_0 t)]. \end{aligned} \quad (2.25)$$

We can easily show that the free boundary conditions are satisfied (the method of mirror images). The response function (2.25) is identical to the

solution which we obtained in §2.1, (2.12). As we can see from this example, the normal mode representation and Schrödinger's solutions are complimentary to each other.

2.3 An Analogy between the Harmonic Lattices and Electrical Circuits

There is a one-to-one correspondence between the harmonic lattice and electrical low pass filter (L-C ladder circuit) as has been discussed by many authors, for example L. Brillouin.⁽²²⁾ It is often very convenient to consider an equivalent electrical circuit of a dynamical system; especially the notion of impedance in the former enables us to skip some of the lengthy calculation. As an example we will consider Schrödinger's solution here. Table 2.2 summarizes the correspondence. The normal modes of an electric circuit such as a low pass filter may be obtained by looking at the zeroes of the impedance. Hence the normal modes of the corresponding dynamical system are easily obtained by simple substitution. The impedance is also very useful when we consider the wave reflection at an impurity in the harmonic lattices. This is a problem of impedance matching in electrical circuits. But we will not go any further in detail on this subject. Refer to van der Pal⁽²⁶⁾

2.4 Heat Flux and Temperature Calculation for Semi-infinite Harmonic Lattices

As a simple application of Schrödinger's solutions we calculate the heat flux and the temperature distribution of the semi-infinite harmonic lattices which we discussed in §2.2. We suppose that only the atom at the end of the lattice interacts with the heat reservoir; it receives random impulses from the reservoir. The approach we take here follows of Uhlenbeck and Ornstein in their classical work on Brownian motion.⁽²⁷⁾

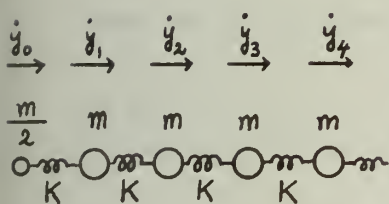
Table 2.2

Dynamical System	Electric Circuit
u_n : difference of the displacement of two neighboring atoms (i.e., $y_{n-1} - y_n$)	V_n : voltage of the n^{th} capacitor
$S_n = \frac{1}{K} \frac{dy_n}{dt}$: velocity of n^{th} atom	I_n : current through n^{th} inductance
m : mass of the atom	L : inductance
k : spring constant	C^{-1} : (reciprocal of) capacitance
<u>boundary</u>	
free end on the left	short circuit on the left
$\omega_0 = 2\sqrt{K/m}$	$\omega_0 = 2/\sqrt{LC}$
<u>initial condition</u>	
$y_0(t) = v_0/2K\delta(t)$	$V_0 = E_0\delta(t)$
<u>equations</u>	
$1/K du_n/dt = S_{n-1} - S_n$	$C dV_n/dt = I_{n-1} - I_n$
$m dS_n/dt = u_n - u_{n+1}$	$L dI_n/dt = V_n - V_{n+1}$
<u>solution</u>	
$S_n(t) = v_0/KJ_{2n}(\omega_0 t)$	$I_n(t) = 2E_0/L J_{2n}(\omega_0 t)$
or	
$\dot{y}_n(t) = v_0 J_{2n}(\omega_0 t)$	

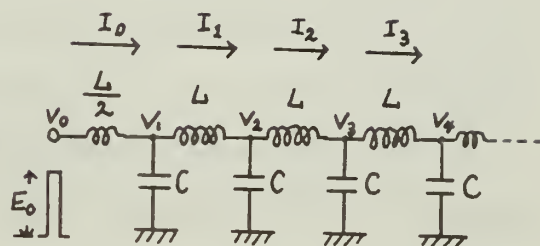
Table 2.2 (continued)

impedance

$$Z(\omega) = \sqrt{mK} \sqrt{1 - \left(\frac{\omega}{\omega_0}\right)^2}$$



$$Z(\omega) = \sqrt{\frac{L}{C}} \sqrt{1 - \left(\frac{\omega}{\omega_c}\right)^2}$$



We have obtained the velocity response function in §2.2:

$$\begin{aligned} F_n(\omega_o t) &= J_{2n}(\omega_o t) + J_{2n+2}(\omega_o t) \\ &= 2(2n+1) J_{2n+1}(\omega_o t) / \omega_o t. \end{aligned} \quad (2.23)$$

The velocity of the n^{th} atom at time t is therefore given as

$$\dot{y}_n(t) = \int_{-\infty}^t f(\tau) F_n(\omega_o(t-\tau)) d\tau \quad (2.26)$$

where $f(\tau)$ is the random function which is characterized by $\overline{f(\tau)}=0$ and $\overline{f(\tau) f(\tau')} = A\delta(\tau-\tau')$. $\overline{(\quad)}$ means the phase average of the variable given in the parentheses. Since the effect of any initial condition is supposed to have propagated toward $n=+\infty$ by the time we observe such ensemble of lattices at time t (actually amplitude and velocity of each atom damp approximately as $(\omega_o t)^{-1/2}$), we only consider the response of each atom of lattices due to the random forces acting on the 0^{th} atom during the time interval $(-\infty, t)$. A constant A has the dimension of $(LT^{-2})^2$ and is to be determined later to make the temperature of the end atom $kT/2m$. By using an explicit form of $F_n(t)$ in (2.23), we can calculate the phase-averaged squared-velocity for each n as:

$$\begin{aligned} \overline{\dot{y}_n(t)^2} &= \int_{-\infty}^t d\tau \int_{-\infty}^t d\tau' f(\tau) f(\tau') F_n(\omega_o(t-\tau)) F_n(\omega_o(t-\tau')) \\ &= A/\omega_o^2 \int_{-\infty}^t F_n^2(\omega_o(t-\tau)) d\omega_o \tau \\ &= A/\omega_o^2 \int_0^\infty F_n^2(s) ds \quad (s = \omega_o(t-\tau)) \\ &= A/\omega_o^2 \frac{4(2n+1)^2 J_{2n+1}^2}{s^2} ds \end{aligned}$$

$$\begin{aligned}
&= \frac{4A(2n+1)^2 \Gamma(2n+1/2)}{\omega_o^2 2^2 \Gamma(3/2) \Gamma(3/2) \Gamma(2n+1+3/2)} \\
&= \frac{A(2n+1)^2 / \pi \omega_o^2}{(2n+1)^2 - 1/4}, \quad (2.27)
\end{aligned}$$

where the phase average is taken at time t over an ensemble of lattices (a large number of similar but independent lattices), which have started at $t=-\infty$ with identical initial conditions given to the corresponding atoms therein, and we have also made use of the following formula⁽²⁵⁾

$$\int_0^\infty \frac{J_m(t) J_n(t)}{t^\lambda} dt = \frac{\Gamma(\lambda) \Gamma((m+n-\lambda+1)/2)}{2^\lambda \Gamma((\lambda+m-n+1)/2) \Gamma((\lambda+n-m+1)/2) \Gamma((m+n+\lambda+1)/2)}. \quad (2.28)$$

We can determine the constant A from the condition $\overline{\dot{y}_o^2}(t) = kT/m$, that is,
 $A = 3\pi\omega_o^2 kT/4m$ or

$$\overline{f(\tau)f(\tau')} = 3\pi\omega_o^2 kT/4m \delta(\tau-\tau').$$

Fig. 2.4 shows the temperature distribution. There is a slight decrease of the temperature near the end atom, then the temperature becomes almost uniform. This tendency is not changed if we define the temperature of each atom by the total energy instead of kinetic energy. The heat flux (instantaneous flux at each point of the lattice) is obtained by using the following formula⁽²¹⁾:

$$J_H(n) = -K(\dot{y}_n + \dot{y}_{n+1})(y_{n+1} - y_n)/2. \quad (2.29)$$

We can obtain the first term immediately from (2.23):

$$(\dot{y}_n + \dot{y}_{n+1})/2 = \int_{-\infty}^t f(\tau) (J_{2n}(\omega_o t) + 2J_{2n+2}(\omega_o t) + J_{2n+4}(\omega_o t)) d\tau/2. \quad (2.30)$$

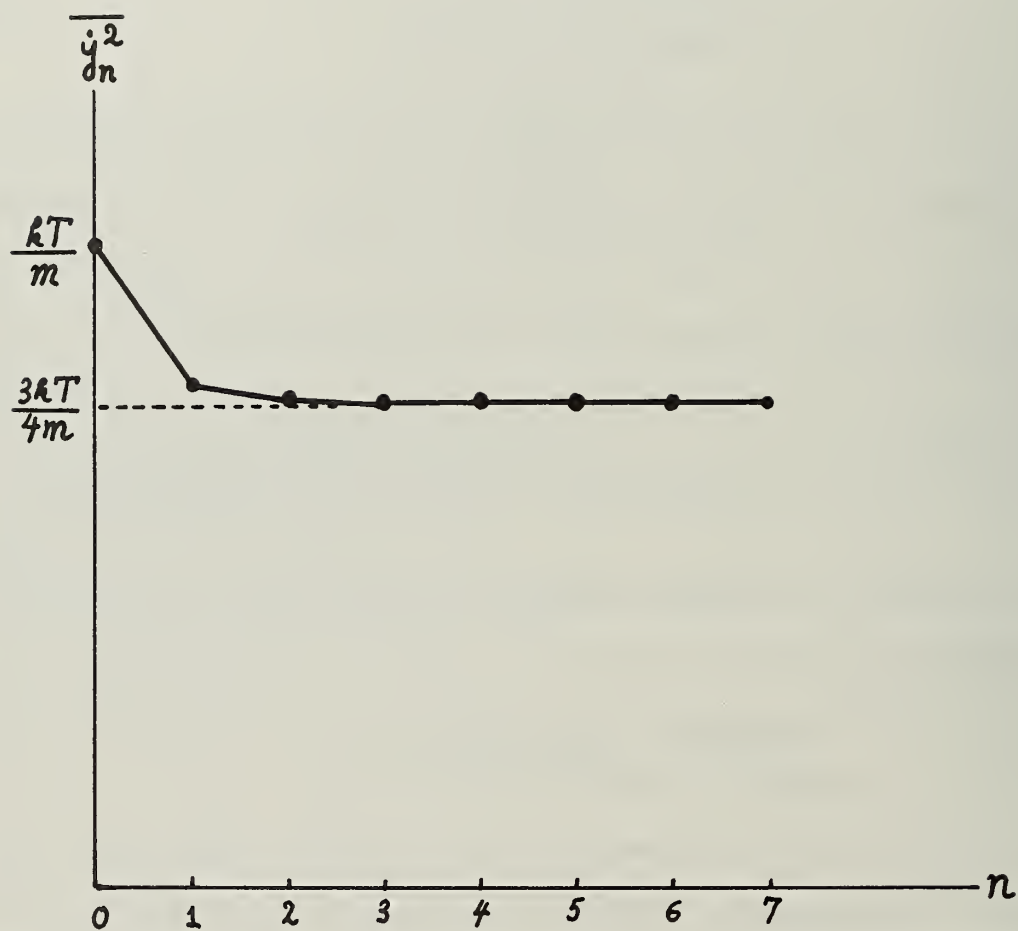


Fig. 2.4. Temperature distribution for semi-infinite lattice.

To calculate the second term we have to define the response function $G_n(t)$ for $y_{n+1} - y_n$. From (2.24) we define

$$G_n(\omega_o t) = - \frac{8(n+1)}{\omega_o} \frac{J_{2n+2}(\omega_o t)}{\omega_o t}. \quad (2.31)$$

Unlike $F_n(\omega_o t)$ this function has the dimension of time. Using $G_n(\omega_o t)$ we can obtain the second term as a convolution form:

$$y_{n+1}(\omega_o t) - y_n(\omega_o t) = \int_{-\infty}^t f(\tau) G_n(\omega_o(t-\tau)) d\tau. \quad (2.32)$$

Substituting (2.30) and (2.32) into (2.29) yields

$$\begin{aligned} J_H(n) &= \frac{4(n+1)AK}{\omega_o} \left(\int_{-\infty}^t f(\tau) (J_{2n}(\omega_o t) + 2J_{2n+2}(\omega_o t) + J_{2n+4}(\omega_o t)) d\tau \right) \\ &\times \left(\int_{-\infty}^t f(\tau') \frac{J_{2n+2}(\omega_o(t-\tau'))}{\omega_o(t-\tau')} d\tau' \right) \end{aligned} \quad (2.33)$$

where we have neglected the effect of initial conditions as before. Taking the phase average and changing the variable $\omega_o(t-\tau)=s$ yield

$$\begin{aligned} \overline{J_H(n)} &= \frac{4(n+1)aAK}{\omega_o^3} \int_0^\infty \left(\frac{J_{2n}(s)J_{2n+2}(s)}{s} \right) + \frac{2J_{2n+2}^2(s)}{s} + \frac{J_{2n+2}(s)J_{2n+4}(s)}{s} ds \\ &= \frac{6\pi kT(n+1)K}{m\omega_o} \int_0^\infty \frac{J_{2n+2}^2(s)}{s} ds \\ &= \frac{3\pi kTK}{2m\omega_o} \\ &= \frac{3\pi kT\omega_o}{8}, \end{aligned} \quad (2.34)$$

where we have made use of the formula (2.28) for $\lambda=1$, or more precisely,

$$\int_0^\infty \frac{J_m(t) J_n(t)}{t} dt = \frac{2 \sin((m-n)\pi/2)}{(m^2-n^2)\pi} = 0 \quad \text{if } m-n: \text{ even}$$

and

$$\int_0^{\infty} \frac{J_m^2(t)}{t} dt = \frac{1}{2m}.$$

Hence a constant heat flux exists. Since the temperature distribution becomes more and more uniform as n increases, it is obvious that Fourier's law of heat conduction does not hold in this case: we cannot define the thermal conductivity! Similar results have been obtained by several authors for different boundary conditions and different thermal situations. (28), (29)

The results obtained in this section entirely depends on the fact that the integral $\int_0^{\infty} F_n^2(t) dt$ converges. That is, the energy fed by the random force to the left atom is transferred to other atoms at a proper rate. As for classical problem of the Brownian particle (Langevan equation) the energy fed from the random force is dissipated by the viscosity so that there is no accumulation of energy in the Brownian particle. If we consider the Schrödinger's lattice, for which the velocity response function is given as $F_n(t) = J_{2n}(\omega_0 t)$ (suppose that the 0^{th} atom interacts with the heat reservoir), the temperature of each atom rises indefinitely since the integral $\int_0^{\infty} J_{2n}^2(\omega_0 t) dt$ diverges for all n . Such catastrophe also occurs for the harmonic lattice of finite length if there is no dissipation of energy.

CHAPTER 3. THE ANHARMONIC LATTICES--CONTINUUM APPROXIMATION AND TODA'S EXACT SOLUTIONS

We can approximate the system of nonlinear ordinary differential equations (1.1) by a nonlinear partial differential equation, provided that the relative displacement of any two neighboring atoms is not large. In the first part of this chapter we will treat such approximation and summarize two special solutions. These solutions have their complete analogues in the water wave theory, in which they are called the cnoidal wave (periodic solution)⁽⁸⁾ and the solitary wave (localized solution).⁽⁶⁾ A new name "Soliton" is frequently used for the latter because of its particle-like behavior (due to Zabusky⁽⁴⁾).

We start from the equation of motion

$$\frac{d^2}{dt^2} y_n = f(y_{n+1} - y_n) - f(y_n - y_{n-1}) . \quad (3.1)$$

We assume that $f(x) \approx x$ when $x \approx 0$, that is, when the lattice is near its natural length.

Historically, Zabusky and Kruskal were the first to introduce the continuum approximation to (3.1).⁽⁹⁾ They reduced (3.1) to a partial differential equation for $y(x,t)$, which is equivalent to (3.5). Then they reduced it into the KdV equation by considering the waves which propagate in one direction (say, in the positive direction). Since the equation (3.5) has solutions which are similar to those in the KdV equation and (3.5) can also describe the waves which travel in the opposite direction, we will use (3.5) as our basic equation. Recently, Wadati and Toda showed that the two solitary wave solutions of both equations give a very good agreement. Readers are referred to (30) and references therein for the KdV equation.

In §3.1, §3.2 and §3.3, we will consider the polynomial type force function, specifically the quadratic nonlinearity and the cubic nonlinearity, for which we can find the analytic solutions. We will show that both the periodic wave and the solitary wave can exist. For the heat conduction problem, the periodic solution is quite irrelevant. But it will also be treated in full since it seems to be the fundamental solution, of which the solitary wave is a special case. For example, only the periodic wave can exist as a travelling wave solution under certain conditions.

In §3.4 we will simplify the force function by introducing the piecewise-linear approximation. We will show that the essential features of the solutions obtained in §3.2 and §3.3 are still retained in this approximation. By this model we can explain why and when the solitary wave solution is possible.

The contents of §3.4 has not been discussed before. In §3.5 we will summarize Toda's solutions for the exponential lattice.

3.1 Polynomial Type Force Function

In the following sections we will consider a cubic polynomial

$$f(x) = x + \alpha x^2 + \beta x^3 \quad (3.2)$$

for the force function. It is more convenient to introduce the relative displacement of two neighboring atoms $u_n = y_{n+1} - y_n$ instead of y_n itself.

Then the equation of motion for u_n is obtained from (3.1) as

$$\frac{d^2}{dt^2} u_n = f(u_{n+1}) - 2f(u_n) + f(u_{n-1}) . \quad (3.3)$$

We will denote the spatial coordinate by x in the continuum approximation.

Then we have

$$u_{n+1} = u_{x=n} + h \left(\frac{\partial u}{\partial x} \right)_{x=n} + \frac{h^2}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_{x=n} + \frac{h^3}{6} \left(\frac{\partial^3 u}{\partial x^3} \right)_{x=n} + \frac{h^4}{24} \left(\frac{\partial^4 u}{\partial x^4} \right)_{x=n} + \dots \quad (3.4)$$

where h is the interatomic distance in equilibrium. Substituting (3.4) into (3.3) with (3.2) yields

$$\ddot{u} = h^2 u'' + 2\alpha h^2 (uu'' + u'^2) + 3\beta h^2 (u^2 u'' + 2uu'^2) + \frac{h^4}{12} u'''' + \dots$$

where $\dot{}$ means the time derivative and $'$ means the spatial derivative.

Putting $h^2 = C_o^2$, $\epsilon C_o^2 = 2\alpha h^2$, $3\beta h^2 = \mu C_o^2$ and $\kappa = \frac{h^4}{12} = \frac{C_o^4}{12}$,

$$\ddot{u} = C_o^2 [u'' + \epsilon (uu')' + \mu (u^2 u')'] + \kappa u'''' \quad (3.5)$$

In order to consider the travelling wave solution, we put

$$u(x, t) = w(x - vt) \equiv w(z)$$

where v is the propagation velocity of the wave (the phase velocity in case of periodic solution) which is to be determined in relation to the amplitude and other factors. Then (3.5) yields

$$(v^2 - C_o^2)w'' = \kappa w'''' + \frac{\epsilon C_o^2}{2} (w^2)'' + \frac{\mu C_o^2}{3} (w^3)''$$

Here $'$ means the derivative with respect to z . Integrating both hand sides twice yields

$$w'' = -\frac{\mu C_o^2}{3\kappa} w^3 - \frac{\epsilon C_o^2}{2\kappa} w^2 + \frac{v^2 - C_o^2}{\kappa} w - \frac{C'}{\kappa} z - \frac{D'}{\kappa} \quad (3.6)$$

where C' and D' are the integration constants. We eliminate the term

$-\frac{C'}{\kappa} z$ since it contains z and is regarded as a spurious term which appeared in the process of integration. This can also be verified by approximately (3.1) by a nonlinear partial differential equation for y and comparing its integrated form (in which w corresponds to $\frac{\partial y}{\partial z}(z)$) with (3.6). So we adopt (3.6) with $C' = 0$. Multiplying (3.6) by w' and integrating with regard to

z once yield

$$(w')^2 = - \frac{\mu C_o^2}{6\kappa} w^4 - \frac{\epsilon C_o^2}{3\kappa} w^3 + \frac{v^2 - C_o^2}{\kappa} w^2 + Dw + E \quad (3.7)$$

where $D = - \frac{2D'}{\kappa}$ and $E = 2E'$ are the new integration constants. The right hand side of (3.7) will be denoted by $P(w)$. We will find the solutions of (3.7) in the following sections. An emphasis will be put, whenever the periodic solution is obtained, on the wave for which the average over its period vanishes ($\bar{w} = 0$). Such wave motion takes place around the equilibrium positions of atoms when the crystal lattice is of natural length. If the external force is applied to the lattice so that it is either compressed or expanded, a periodic wave is set on around the new equilibrium length. This corresponds to considering a solution for which $\bar{w} \neq 0$; $\bar{w} > 0$ for the expanded lattice (to be called "positive background") and $\bar{w} < 0$ for the compressed lattice ("negative background"). The propagation velocity of the waves under such circumstances differs from that of the waves in the lattice of natural length due to the nonlinearity of the force function.

As for the solitary wave solution, we are most interested in the one for which the lattice is of natural length at $z = \pm \infty$. This means that the energy is concentrated at the wave front. (Fig. 3.1) We call such wave zero-back ground wave.

3.2 Quadratic Nonlinearity ($\mu=0$, $\epsilon \neq 0$)

The equation (3.8) yields, in this case

$$\left(\frac{dw}{dz}\right)^2 = - \frac{\epsilon C_o^2}{3\kappa} w^3 + \frac{v^2 - C_o^2}{\kappa} w^2 + Dw + E \equiv P(w). \quad (3.8)$$

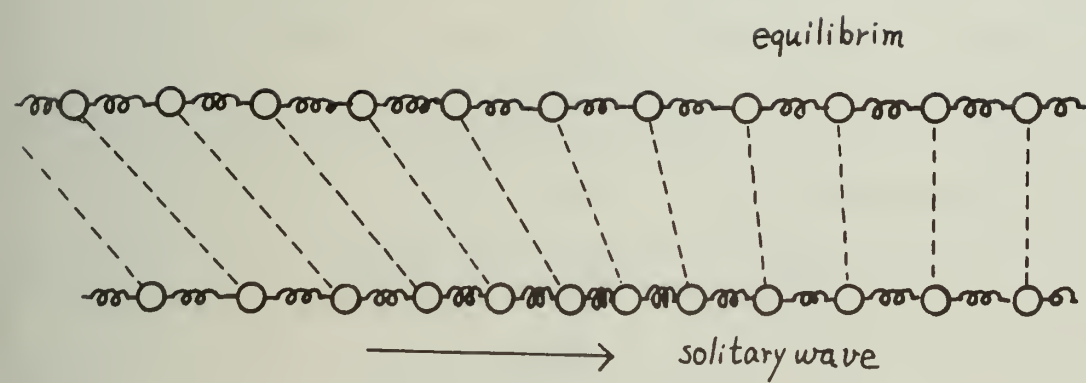


Fig. 3.1. Solitary wave on zero background.

3.2.1 $\varepsilon > 0$ Periodic Wave

We consider the case in which $P(w)$ has three distinct real roots:

$$P(w) = \rho^2 (a-w)(w-b)(w-c) \quad (a > b > c)$$

where

$$\rho^2 = \frac{\varepsilon C_o^2}{3\kappa}, \quad \rho^2 (a+b+c) = \frac{v^2 - C_o^2}{\kappa}.$$

Then we have a bounded solution in $[b, a]$ (Fig. 3.2) which may be expressed in terms of the Jacobian elliptic functions as

$$w(z) = a - (a-b) \operatorname{sn}^2 \left(\frac{\sqrt{a-c}}{2} \rho z, k \right) = c + (a-c) \operatorname{dn}^2 \left(\frac{\sqrt{a-c}}{2} \rho z, k \right)$$

where $k^2 = \frac{a-b}{a-c}$ is the modulus of the elliptic function.* Going back to x, t coordinates, we have

$$u(x-vt) = a - A \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right) \quad (3.9a)$$

$$= c + \frac{A}{k^2} \operatorname{dn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right) \quad (3.9b)$$

where

$$A = a - b \quad (\text{amplitude})$$

$$k_x = \frac{\pi C_o}{4Kk} \sqrt{\frac{\varepsilon}{3\kappa}} A \quad (\text{wave number})$$

$$\omega = v \cdot k_x \quad (\text{frequency})$$

and

$$K = K(k) \quad (\text{the complete integral of first kind}).$$

The velocity v is given in terms of a, b, c from the quadratic term in (3.8):

$$\frac{v^2 - C_o^2}{\kappa} = \rho^2 (a+b+c) = \frac{\varepsilon C_o^2}{3\kappa} (a+b+c)$$

or

$$v^2 = C_o^2 \left(1 + \frac{\varepsilon}{3} (a+b+c) \right). \quad (3.10)$$

* See Appendix B for collections of solutions.

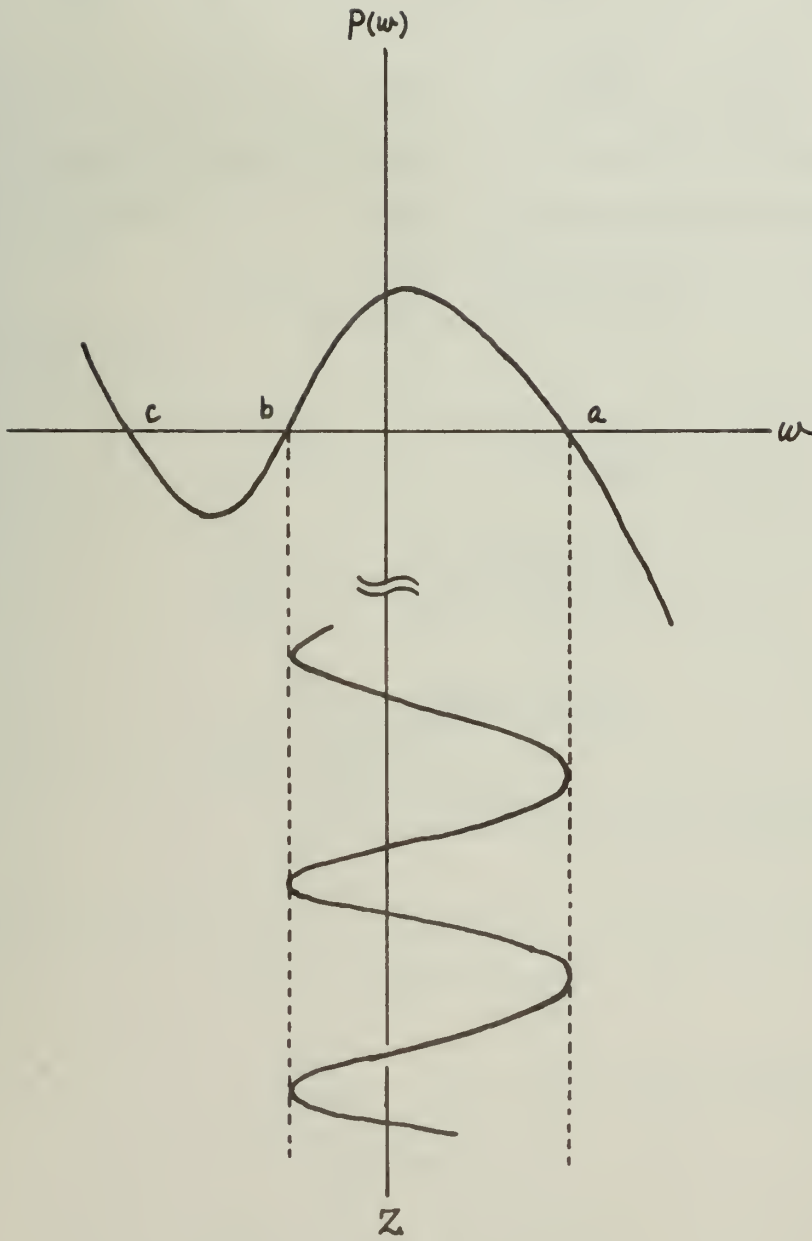


Fig. 3.2. Quadratic nonlinearity ($\epsilon > 0$): periodic wave.

Note that $v > C_0$ if $a+b+c > 0$ and vice versa. The periodic solution is completely determined by three zeroes of $P(w)$. If we further assume the zero background wave, we have the two parameter family solutions, for which A , k_x , ω and k are explicitly related. First we should note that

$$\frac{1}{2K} \int_0^{2K} \text{sn}^2 x dx = \frac{1}{2K} \int_0^{2K} \frac{1}{k^2} (1 - \text{dn}^2 x) dx = \frac{1}{k^2} \left(1 - \frac{E(k)}{K(k)}\right)$$

since $Z(x) = \int_0^x \text{dn}^2 x - \frac{E(k)}{K(k)} x$ is periodic of period $2K$ (Zeta elliptic function of Jacobi). Here $E(k)$ is the complete elliptic integral of the second kind. Using the above relation, we have

$$\bar{u} = a - A \overline{\text{sn}^2} = a - \frac{A}{k^2} \left(1 - \frac{E}{K}\right) = 0$$

or

$$a = \frac{A}{k^2} \left(1 - \frac{E}{K}\right).$$

Therefore

$$\begin{aligned} u(x-vt) &= \frac{A}{k^2} (\text{dn}^2(\frac{2K}{\pi}(k_x x - \omega t)) - \frac{E}{K}) \\ &= \frac{A}{k^2} \frac{d}{dz} Z(z) \Big|_{z = \frac{2K}{\pi}(k_x x - \omega t)}. \end{aligned}$$

From the definition of A and k^2 , we also have

$$b = a - A$$

$$c = a - \frac{A}{k^2}.$$

Substituting a, b, c into (3.10) yields

$$\begin{aligned} v^2 &= C_0^2 \left(1 + \frac{\varepsilon}{3} \left(3a - A - \frac{A}{k^2}\right)\right) \\ &= C_0^2 \left(1 + \frac{\varepsilon}{3} \left(\frac{3A}{k^2} - \frac{3AE}{k^2 K} - A - \frac{A}{k^2}\right)\right) \\ &= C_0^2 \left(1 + \frac{\varepsilon A}{3k^2} \left(2 - k^2 - \frac{3E}{K}\right)\right). \end{aligned} \tag{3.11}$$

Hence the velocity of the periodic waves can become either "supersonic"

($v > C_0$) or "subsonic" ($v < C_0$) depending on the degree of deformation

(i.e. the modulus k). The critical modulus k_c is given by solving

$\frac{3E(k)}{K(k)} = 2 - k^2$, for which $v = C_0$ holds independent of the amplitude A . Approximately $k_c \simeq .98$.

The dispersion relation for zero background wave is

$$\omega^2 = v^2 k_x^2 = C_0^2 \left(1 - \frac{\epsilon}{3} A\right) k_x^2 - \mu \left(\frac{4K}{\pi}\right)^2 \left(\frac{3E}{K} - 2\right) k_x^4.$$

If $k \rightarrow 0$ and $\frac{A}{k^2}$ finite, $\omega^2 = C_0^2 k_x^2 - 4\mu k_x^4$ (dispersive harmonic wave) and

if $k \rightarrow 1$ $\omega^2 = C_0^2 k_x^2 \left(1 + \frac{\epsilon A}{3}\right)$ (approaches to solitary wave).

Solitary Wave

If b approaches to c , we have the solitary wave solution. Since

$k^2 = \frac{a-b}{a-c} \rightarrow 1$, $dn^2 \rightarrow \text{sech}^2$. In this limit (3.9b) reduces to

$$u(x-vt) = b + A \text{sech}^2(\alpha x - \beta t) \quad (3.12a)$$

where

$$A = a - b$$

$$\alpha = \frac{\sqrt{a-b}}{3\mu} = \sqrt{\frac{\epsilon A}{12\mu}}$$

$$v^2 = C_0^2 \left(1 + \frac{\epsilon}{3}(a+2b)\right) \quad (3.12b)$$

and

$$\beta = \alpha \cdot v.$$

Consider the zero-background solitary wave, i.e. $b = 0$. Then

$$u(x-vt) = A \text{sech}^2(\alpha x - \beta t) \quad (3.13a)$$

where

$$\alpha = \sqrt{\frac{\epsilon A}{12\mu}}$$

$$v^2 = C_0^2 \left(1 + \frac{\epsilon}{3} A\right) \quad (3.13b)$$

and

$$\beta = \alpha \cdot v.$$

Note that the solitary wave is always created toward the positive w direc-

tion. Since $u_n = y_{n+1} - y_n > 0$, this means that only rarefactive solitary

wave is possible for $\epsilon > 0$.

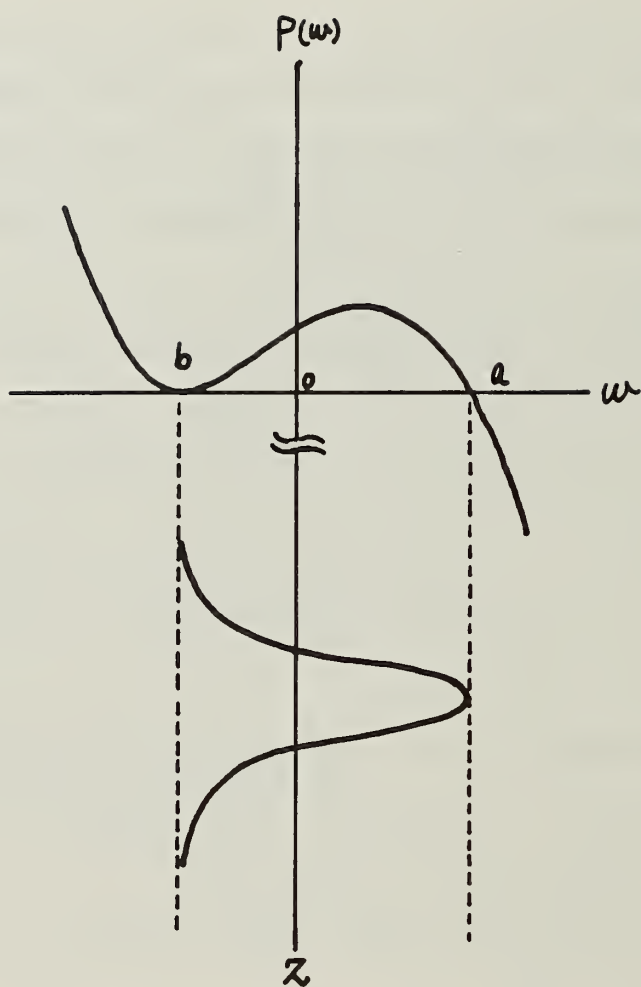


Fig. 3.3. Quadratic nonlinearity ($\varepsilon > 0$): solitary wave.

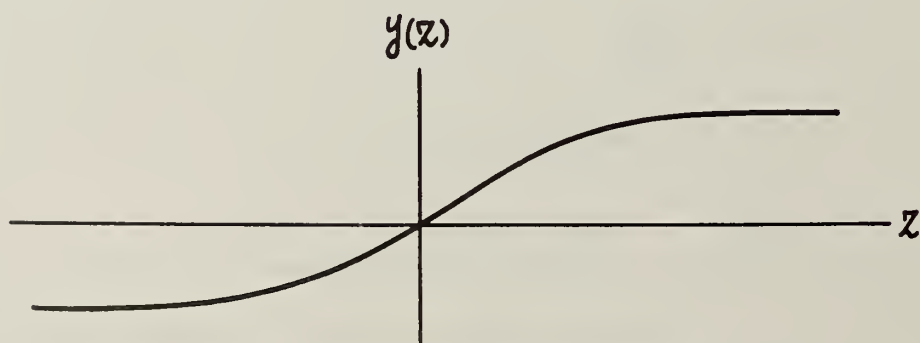


Fig. 3.4. A typical profile of solitary wave.

3.2.2 $\varepsilon < 0$

The derivation of solutions for the negative ε is almost identical to 3.2.1. The equation (3.7) yields

$$\left(\frac{dw}{dz}\right)^2 = \rho^2 (a-w)(b-w)(w-c)$$

where

$$\rho^2 = \frac{|\varepsilon| C_o^2}{3\mu}, \quad \rho^2 (a+b+c) = \frac{v^2 - C_o^2}{\mu}.$$

Obviously bounded solutions exist only in $[c, b]$ (Fig. 3.5).

The periodic solution is:

$$\begin{aligned} w(z) &= c + (b-c) \operatorname{sn}^2\left(\frac{\sqrt{a-c}}{2} \rho z, k\right) \\ &= a - (a-c) \operatorname{dn}^2\left(\frac{\sqrt{a-c}}{2} \rho z, k\right) \\ k^2 &= \frac{b-c}{a-c} \end{aligned}$$

or

$$\begin{aligned} u(x-vt) &= c + A \operatorname{sn}^2\left(\frac{2K}{\pi}(k_x x - \omega t), k\right) \\ &= c + \frac{A}{2} \left\{ 1 - \operatorname{dn}^2\left(\frac{2K}{\pi}(k_x x - \omega t), k\right) \right\} \end{aligned} \quad (3.14)$$

where

$$\begin{aligned} A &= b-c && \text{(amplitude)} \\ k_x &= \frac{\pi C_o}{4kK} \sqrt{\frac{|\varepsilon|}{3\mu}} A && \text{(wave number)} \\ \omega &= vk_x && \text{(frequency)} \\ K &= K(k) \end{aligned}$$

and

$$v^2 = C_o^2 \left(1 - \frac{|\varepsilon|}{3} (a+b+c)\right). \quad (3.15)$$

Obviously the velocity becomes "supersonic" if $a+b+c < 0$, and vice versa.

We can obtain the more explicit (two parameter) solutions for zero background waves ($\bar{u}=0$) by following the same procedure as before.

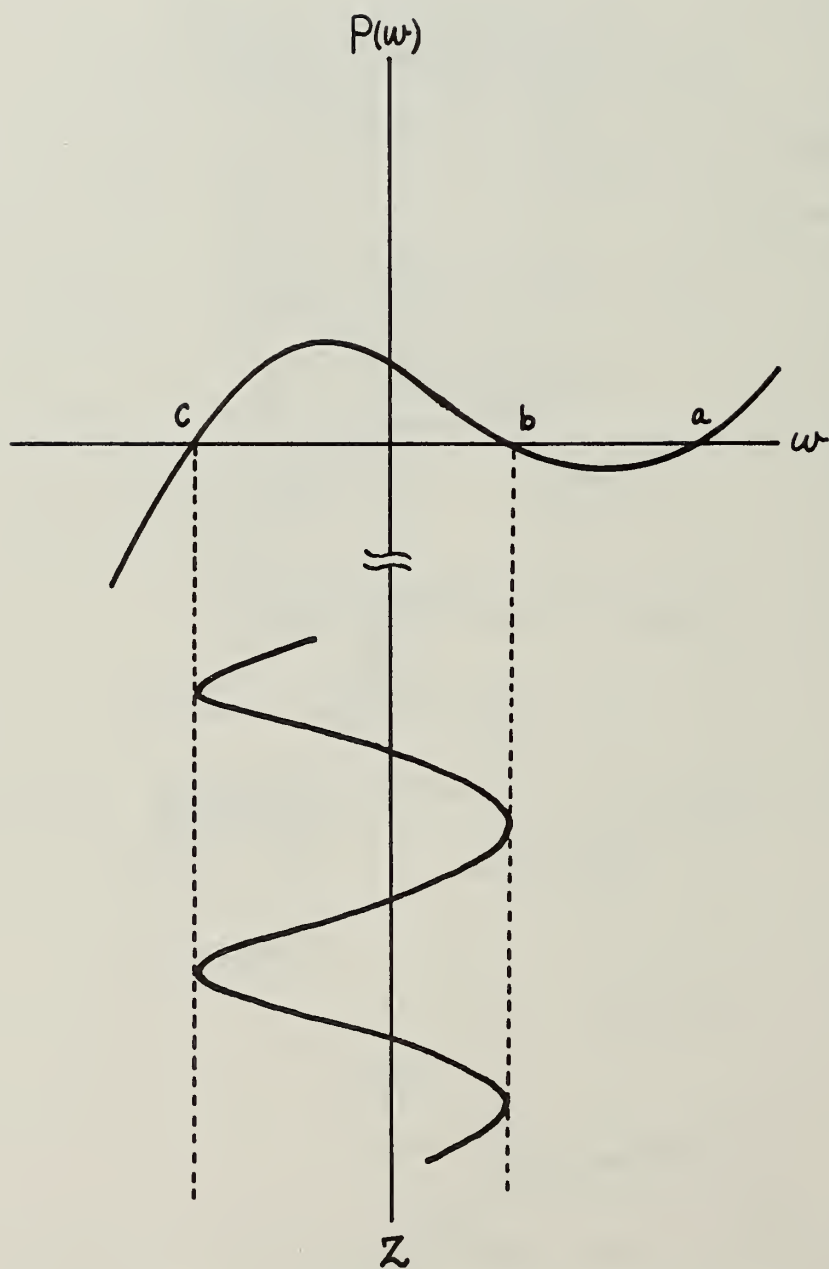


Fig. 3.5. Quadratic nonlinearity ($\varepsilon < 0$): periodic wave.

Results are:

$$u(x-vt) = -\frac{A}{k} \left\{ \operatorname{dn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right) - \frac{E}{K} \right\}$$

$$\omega^2 = C_o^2 \left(1 - \frac{|\epsilon|A}{3k^2} (k^2 + (\frac{3E}{K} - 2)) \right).$$

The critical modulus k_c is also $\simeq .98$. The dispersion relation is

$$\omega^2 = C_o^2 k_x^2 - \kappa \left(\frac{4K}{\pi} \right)^2 (k^2 + \frac{3E}{K} - 2) k_x^4.$$

Hence

$$\text{if } k \rightarrow 0 \text{ and } \frac{A}{k^2} \text{ finite, } \omega^2 = C_o^2 k_x^2 - 4\kappa k_x^4 \text{ and}$$

$$\text{if } k \rightarrow 1, \quad \omega^2 = C_o^2 \left(1 + \frac{|\epsilon|A}{3} \right) k_x^2.$$

Solitary Waves

We also have the solitary wave solution in the limit $a \rightarrow b$ (Fig. 3.6):

$$u(x-vt) = b - A \operatorname{sech}^2(\alpha x - \beta t) \quad (3.16)$$

where

$$A = b - c$$

$$\alpha = \sqrt{\frac{|\epsilon|A}{12\kappa}}$$

$$\beta = \alpha \cdot v$$

$$\text{and} \quad v^2 = C_o^2 \left(1 - \frac{|\epsilon|A}{3} (2b+c) \right). \quad (3.17)$$

For the zero-background wave, ($b=0$)

$$u(x-vt) = -A \operatorname{sech}^2(\alpha x - \beta t) \quad (3.18)$$

where

$$A = -c > 0$$

$$\alpha = \sqrt{\frac{|\epsilon|A}{12\kappa}}$$

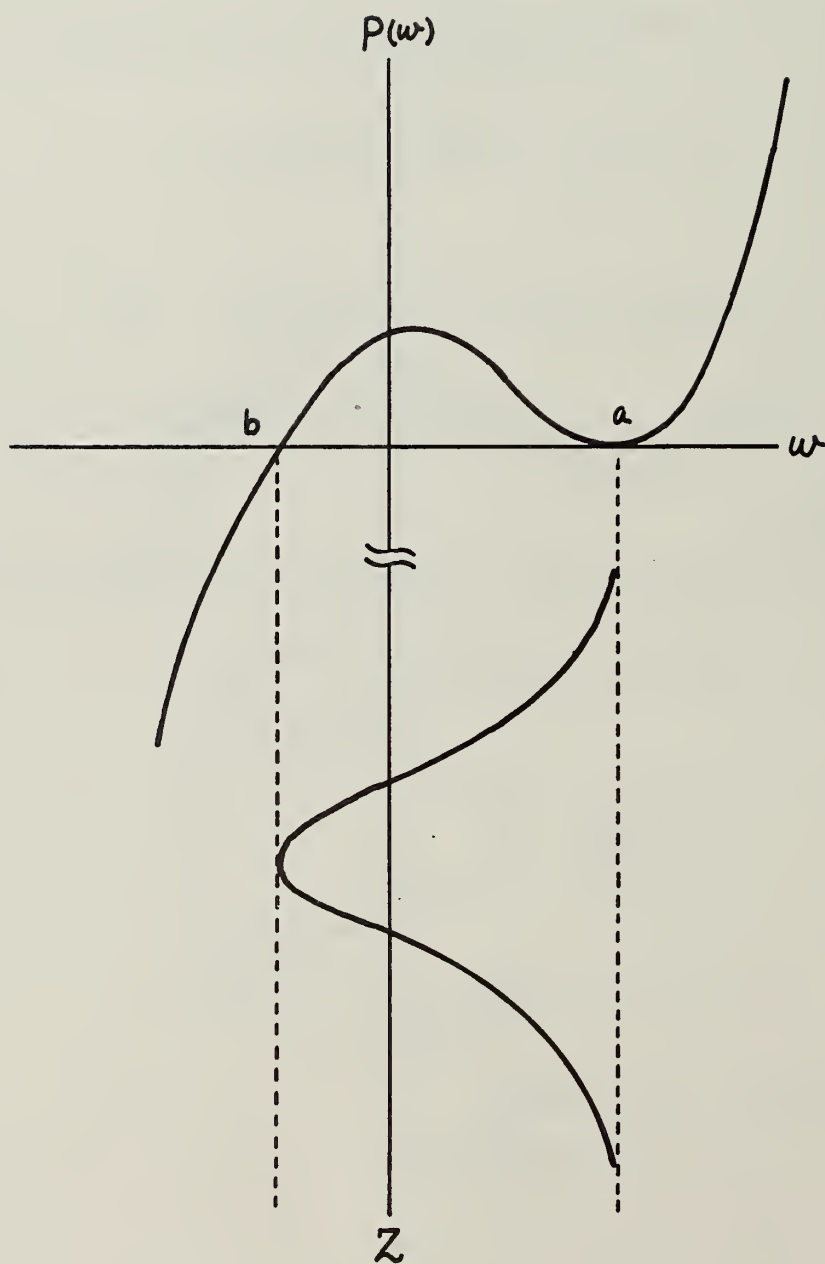


Fig. 3.6. Quadratic nonlinearity ($\varepsilon < 0$): solitary wave.

and

$$v^2 = c_o^2 \left(1 + \frac{\epsilon A}{3}\right). \quad (3.19)$$

Only the compressive solitary wave is possible if $\epsilon < 0$. Combining this result with the one obtained for $\epsilon > 0$, we can summarize that the solitary wave is always created in the region in which the nonlinearity becomes hard. This is one of the common features of the solitary waves.

3.3 Cubic Nonlinearity ($\mu \neq 0$)

We can expect that the higher order nonlinearity will produce more variety in the solutions. We often put $\epsilon=0$ in this section for the sake of simplicity, because the quadratic nonlinearity does not change the nature of the solution. That is, the cubic term in (3.7) can be always absorbed in the quartic term by a simple transformation of variable:

$$\begin{aligned} P(w) &= -\frac{\mu C_o^2}{6\mu} w^4 - \frac{\epsilon C_o^2}{3\mu} w^3 + \frac{v^2 - C_o^2}{\mu} w^2 + Dw + E \\ &= -\frac{\mu C_o^2}{6\mu} \left(w + \frac{\epsilon}{2\mu}\right)^4 + \frac{C_o^2}{\mu} \left(\frac{v^2}{C_o^2} - 1 + \frac{\epsilon^2}{4\mu}\right) \left(2 + \frac{\epsilon}{3\mu}\right) \\ &\quad + D' \left(w + \frac{\epsilon}{2\mu}\right) + E' \end{aligned}$$

where D' , E' are new constants.

It is clear that the existence of the cubic term results in the shifting of the solution and of the velocity.

3.3.1 $\mu > 0$ (Hard Nonlinearity)

Let $P(w) = -\rho^2 (w-a)(w-b)(w-c)(w-d)$ where $\rho^2 = \frac{\mu C_o^2}{6\mu}$. a, b, c, d are the four real roots of $P(w) = 0$ and they satisfy the following equations:

$$a + b + c + d = \frac{\epsilon C_o^2}{3\mu\rho^2} = -\frac{2\epsilon}{\mu} \quad (3.20)$$

$$ab+bc+ca+ad+bd+cd = - \frac{v^2 - c_o^2}{\mu \rho^2} = - \frac{6}{\mu} \left(\frac{v^2}{c_o^2} - 1 \right). \quad (3.21)$$

Periodic Wave

There are two bounded regions in w , for which the periodic solutions exist. They are $[d, c]$ and $[b, a]$ (Fig. 3.7). The periodic solutions are expressed in terms of the Jacobian elliptic functions (see Appendix B):

$$w_I(z) = \frac{d + a \cdot \frac{c-d}{a-c} \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)}{1 + \frac{c-d}{a-c} \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)} \quad d \leq w_I \leq c$$

or

$$u_I(x-vt) = \frac{d + a \cdot \frac{c-d}{a-c} \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)}{1 + \frac{c-d}{a-c} \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)}, \quad (3.22)$$

and

$$w_{II}(z) = \frac{a + d \left(\frac{a-b}{b-d} \right) \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)}{1 + \frac{a-b}{b-d} \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)} \quad b \leq w_{II} \leq a$$

or

$$u_{II}(x-vt) = \frac{a + d \left(\frac{a-b}{b-d} \right) \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)}{1 + \frac{a-b}{b-d} \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)} \quad (3.23)$$

where

$$k^2 = \frac{(a-b)(c-d)}{(a-c)(b-d)} \quad (\text{modulus})$$

$$k_x = \frac{\pi c_o}{4K} \sqrt{\frac{\mu(a-c)(b-d)}{6\mu}}$$

$$\omega = v \cdot k_x$$

and

$$K = K(k) \quad (\text{the elliptic integral of the first kind}).$$

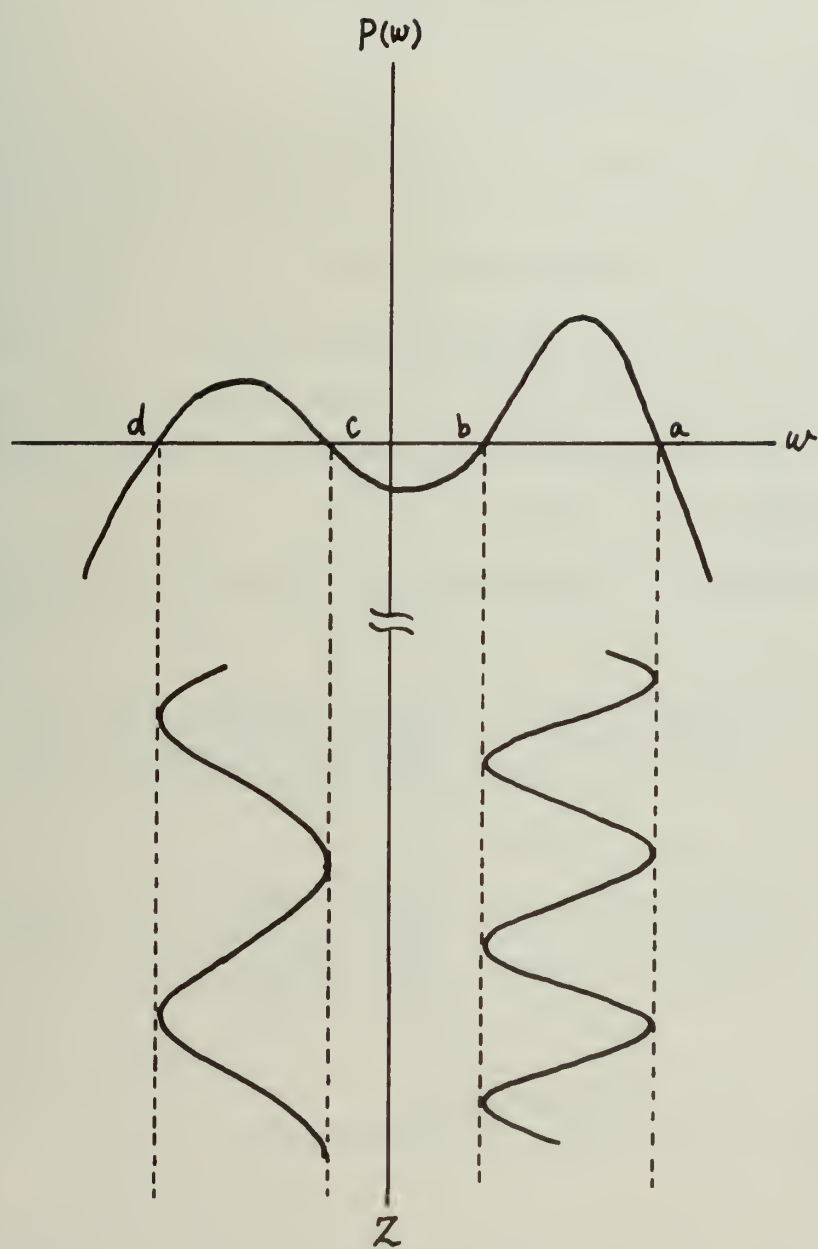


Fig. 3.7. Cubic nonlinearity ($\mu > 0$): periodic waves I.

The velocity is given by (3.20) and (3.21):

$$\begin{aligned}
 v^2 &= C_o^2 \left[1 - \frac{\mu}{6}(ab+bc+ca+ad+bd+cd) \right] \\
 &= C_o^2 \left[1 - \frac{\mu}{12}((a+b+c+d)^2 - (a^2+b^2+c^2+d^2)) \right] \\
 &= C_o^2 \left[1 - \frac{\varepsilon^2}{3\mu} + \frac{\mu}{12}(a^2+b^2+c^2+d^2) \right]. \quad (3.24a)
 \end{aligned}$$

Or, eliminating d completely yields

$$v^2 = C_o^2 \left[1 + \frac{\varepsilon}{3}(a+b+c) + \frac{\mu}{12}\{(a-b)^2 + (b-c)^2 + (c-a)^2\} \right]. \quad (3.24b)$$

If $\varepsilon = 0$, the velocity is always greater than C_o . For a nonzero ε , the condition $\varepsilon^2 - 3\mu < 0$ must hold. This condition guarantees the stability of the lattice; the interaction force is always attractive when the relative displacement is large enough.

Solitary Waves

In the limit $b \rightarrow c$, both solutions (3.22) and (3.23) approach to the solitary waves:

$$U_I(x-vt) = \frac{d+a\frac{b-d}{a-b} \tanh^2(\alpha x - \beta t)}{1 + \frac{b-d}{a-b} \tanh^2(\alpha x - \beta t)} = \frac{\frac{b(a-d)}{a-b} - \frac{a(b-d)}{a-b} \operatorname{sech}^2(\alpha x - \beta t)}{\frac{a-d}{a-b} - \frac{b-d}{a-b} \operatorname{sech}^2(\alpha x - \beta t)} \quad (3.25)$$

and

$$U_{II}(x-vt) = \frac{a+d\frac{a-b}{b-d} \tanh^2(\alpha x - \beta t)}{1 + \frac{a-b}{b-d} \tanh^2(\alpha x - \beta t)} = \frac{\frac{b(a-d)}{b-d} - \frac{d(a-b)}{b-d} \operatorname{sech}^2(\alpha x - \beta t)}{\frac{a-d}{b-d} - \frac{a-b}{b-d} \operatorname{sech}^2(\alpha x - \beta t)} \quad (3.26)$$

where

$$\alpha = \sqrt{\frac{\mu C_o^2}{24u}(a-b)(b-d)}$$

and

$$\beta = v \cdot \alpha.$$

Hence the solitary wave solution in general is an infinite series of $\operatorname{sech}^2(\alpha x - \beta t)$ even in this approximation. If we choose the special value

$b = c = 0$, the above solutions become simple. In this case we can obtain the zero background solutions. Since $a+d = 0$,

$$u_I(x-vt) = -a \cdot \frac{1 - \tanh^2(\alpha x - \beta t)}{1 + \tanh^2(\alpha x - \beta t)} = -a \cdot \operatorname{sech}(2\alpha x - 2\beta t)$$

and

$$u_{II}(x-vt) = a \cdot \operatorname{sech}(2\alpha x - 2\beta t) \quad (3.28)$$

with

$$\alpha = \sqrt{\frac{\mu C_o^2}{24\kappa}} a$$

$$\beta = v\alpha$$

and

$$v^2 = C_o^2 \left(1 + \frac{\varepsilon}{3} a + \frac{\mu}{6} a^2\right). \quad (3.29)$$

Periodic Waves around the Natural Length of Lattice

Since $P(w)$ is a quartic polynomial with the negative leading coefficient, bounded solutions are possible even if $P(w)$ does not have four real zeroes. As a simple example, we will consider the periodic wave which is symmetric around the natural length of the lattice and also $\varepsilon=0$. Such a wave can be realized by putting

$$P(w) = (a^2 - w^2)(w^2 + b^2)\rho^2. \quad (\text{Fig. 3.8})$$

The equation is

$$\left(\frac{dw}{dz}\right)^2 = \rho^2 (a^2 - w^2)(w^2 + b^2), \quad (3.30)$$

solution of which is

$$w(z) = a \operatorname{cn}(\sqrt{a^2 + b^2} \rho z, k), \quad \text{with } k^2 = \frac{a^2}{a^2 + b^2}.$$

(See Appendix B.) Or, in terms of x and t

$$u(x-vt) = a \operatorname{cn}\left(\frac{2K}{\pi}(k_x x - \omega t), k\right) \quad (3.31)$$

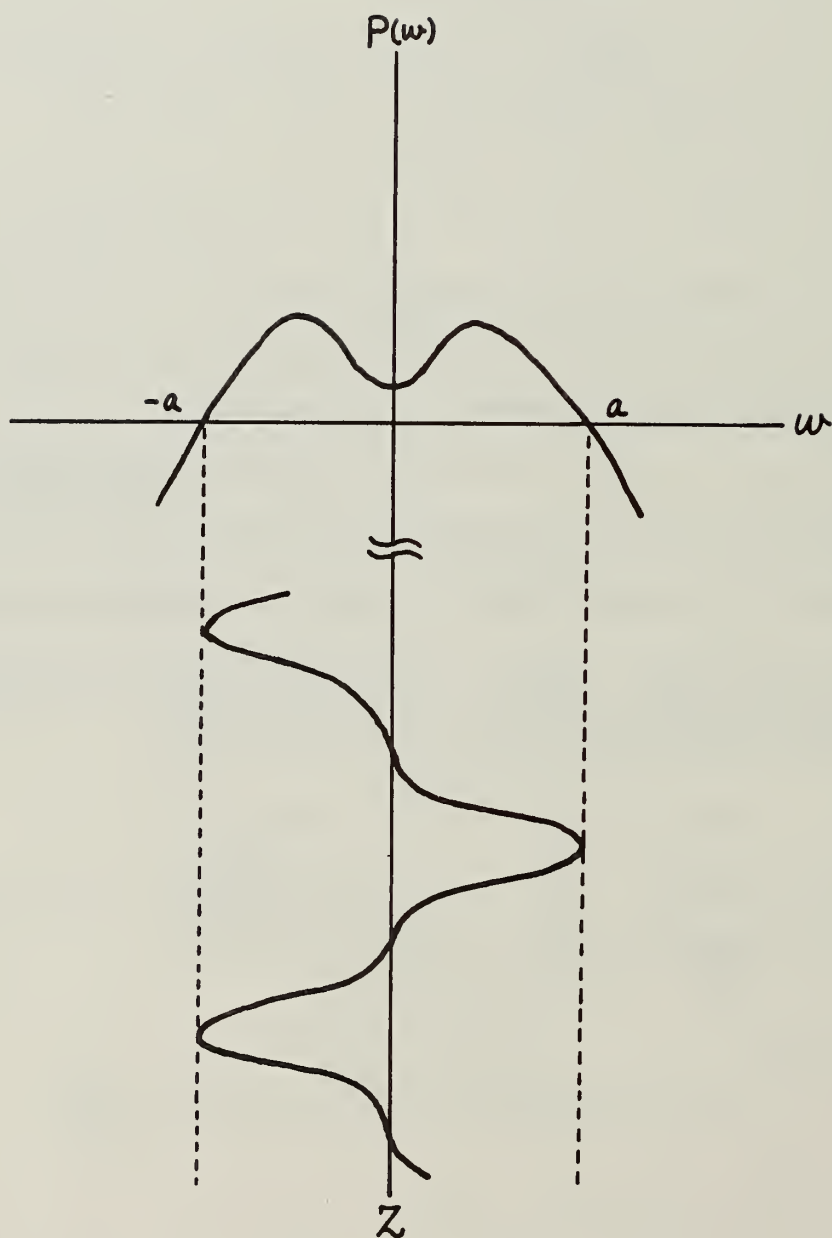


Fig. 3.8. Cubic nonlinearity ($\mu > 0$): periodic wave II (symmetric).

where

$$k_x = \frac{\pi}{2K} \sqrt{\frac{\mu C_o^2}{6\mu} (a^2 + b^2)} = \frac{\pi}{2K} C_o \sqrt{\frac{\mu}{6\mu}} \frac{a}{k}$$

$$\omega = vk_x$$

$$K = K(k) .$$

The velocity is given by the quadratic term in (3.30):

$$\frac{v^2 - C_o^2}{\mu} = \frac{\mu C_o^2}{6\mu} (a^2 - b^2) = \frac{\mu C_o^2}{6\mu} (a^2 - \frac{a^2}{k^2} + a^2) = \frac{\mu C_o^2}{6\mu} a^2 (2 - \frac{1}{k^2})$$

or

$$v^2 = C_o^2 (1 + \frac{\mu a^2}{6} (2 - \frac{1}{k^2})) .$$

Hence the wave is "supersonic" if $k > \frac{1}{\sqrt{2}}$ and "subsonic" if $k < \frac{1}{\sqrt{2}}$. The dispersion relation is

$$\omega^2 = C_o^2 k_x^2 (1 + \frac{\mu}{3} a^2) - \mu (\frac{2K}{\pi})^2 k_x^4 . \quad (3.32)$$

As $a \rightarrow 0$, (3.32) reduces to $\omega^2 = C_o^2 k_x^2 - \mu k_x^4$, the dispersion relation for the linearized equation of (3.5)

$$\ddot{u} = C_o^2 u'' + \mu u'''' .$$

Algebraic Solitary Waves⁽³¹⁾

All the solitary wave solutions discussed so far (both quadratic and cubic case) decay exponentially as $z \rightarrow \pm\infty$. But there is also an extra solution for the cubic nonlinearity which behaves like z^{-2} as $z \rightarrow \pm\infty$. Such a solution exists if $P(w)$ has a triple zero (Fig. 3.9). Namely,

$$\left(\frac{dw}{dz}\right)^2 = \rho^2 (w-a)^3 (b-w) \equiv P(w) \quad (a < b) \quad (3.33)$$

has a solution

$$w(z) = a + \frac{b}{1 + (2b\rho z)^2} . \quad (3.34)$$

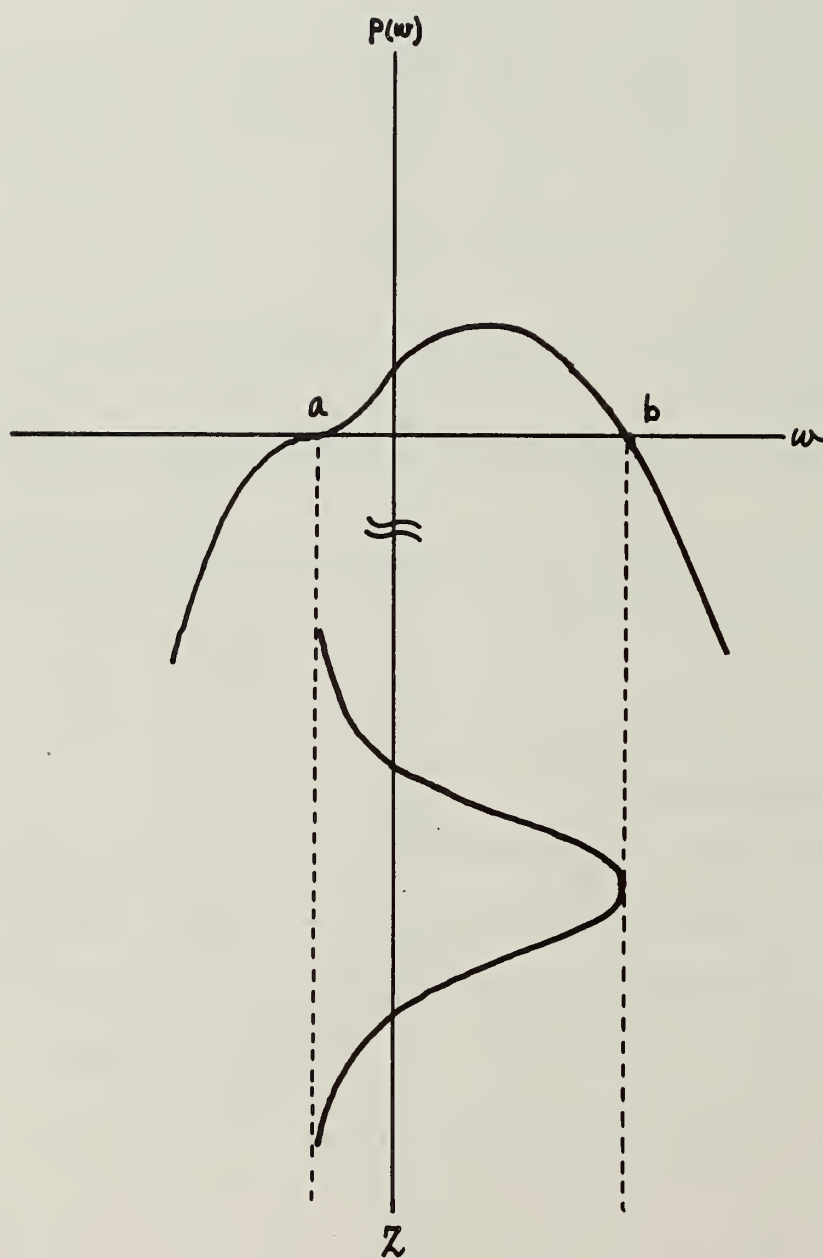


Fig. 3.9. Cubic nonlinearity ($\mu > 0$): algebraic solitary wave.

To simplify the formulation, we assume that $\epsilon=0$. Since

$$P(w) = -\rho^2(w^4 - (3a+b)w^3 + 3a(a+b)w^2 - a^2(a+3b)w + a^3b),$$

we obtain the following equations from the cubic and quadratic terms:

$$\begin{aligned} \rho^2(3a+b) &= -\frac{\epsilon C_o^2}{3\mu} = 0 \\ 3a\rho^2(a+b) &= -\frac{(v_o^2 - C_o^2)}{\mu}. \end{aligned}$$

From the first equation

$$a = -\frac{b}{3}.$$

From the second equation

$$v_o^2 - C_o^2 = \frac{\mu C_o^2}{6} \left(\frac{2}{3} b^2\right).$$

The solution (3.34) may be rewritten in terms of b alone:

$$w(z) = -\frac{b}{3} + \frac{b}{1+(2b\rho z)^2}.$$

If we define the amplitude of the wave as $A = a-b$

$$= \frac{4}{3} b,$$

$$w(z) = \frac{A}{4} \left(-1 + \frac{3}{1 + \frac{3\mu C_o^2}{8\mu} A^2 z^2} \right).$$

The velocity-amplitude relation is

$$v_o^2 = C_o^2 \left(1 + \frac{\mu}{16} A^2 \right).$$

The algebraic solitary wave differs greatly from the ordinary (sech^2 type) solitary waves. The differences are summarized as follows:

- (1) decay is much slower (Lorenzian);
- (2) the amplitude is large and the condition to allow such wave is very strict (triple zero required for $P(w)$).

(3) the wave must cover both the positive and the negative w regions.

In order to obtain the zero background wave, we must introduce the nonzero ϵ , in which case the solution yields

$$w(z) = -\frac{2\epsilon}{\mu} \frac{1}{1 + \frac{2\epsilon^2 C_o^2}{3\mu} z^2}.$$

Hence the amplitude is determined uniquely.

(4) The velocity is slow compared with the ordinary solitary wave of the same height.

Since the algebraic solitary wave exists under very limited conditions, we will exclude this type of solution in the future consideration.

3.3.2 $\mu < 0$ (Soft Nonlinearity)

We can put

$$P(w) = \rho^2 (w-a)(w-b)(w-c)(w-d)$$

where

$$\rho^2 = \frac{|\mu| C_o^2}{3\mu}$$

$$a+b+c+d = \frac{2\epsilon}{|\mu|} \quad (3.36a)$$

$$\rho^2 (ab+bc+cd+da+ac+bd) = \frac{v^2 - C_o^2}{\mu}. \quad (3.36b)$$

Periodic Wave

There is only one region of w in which bounded solutions exist (Fig. 3.10). The solutions are:

$$w_I(z) = \frac{c-d \left(\frac{b-c}{b-d}\right) \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)}{1 - \left(\frac{b-c}{b-d}\right) \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)}$$

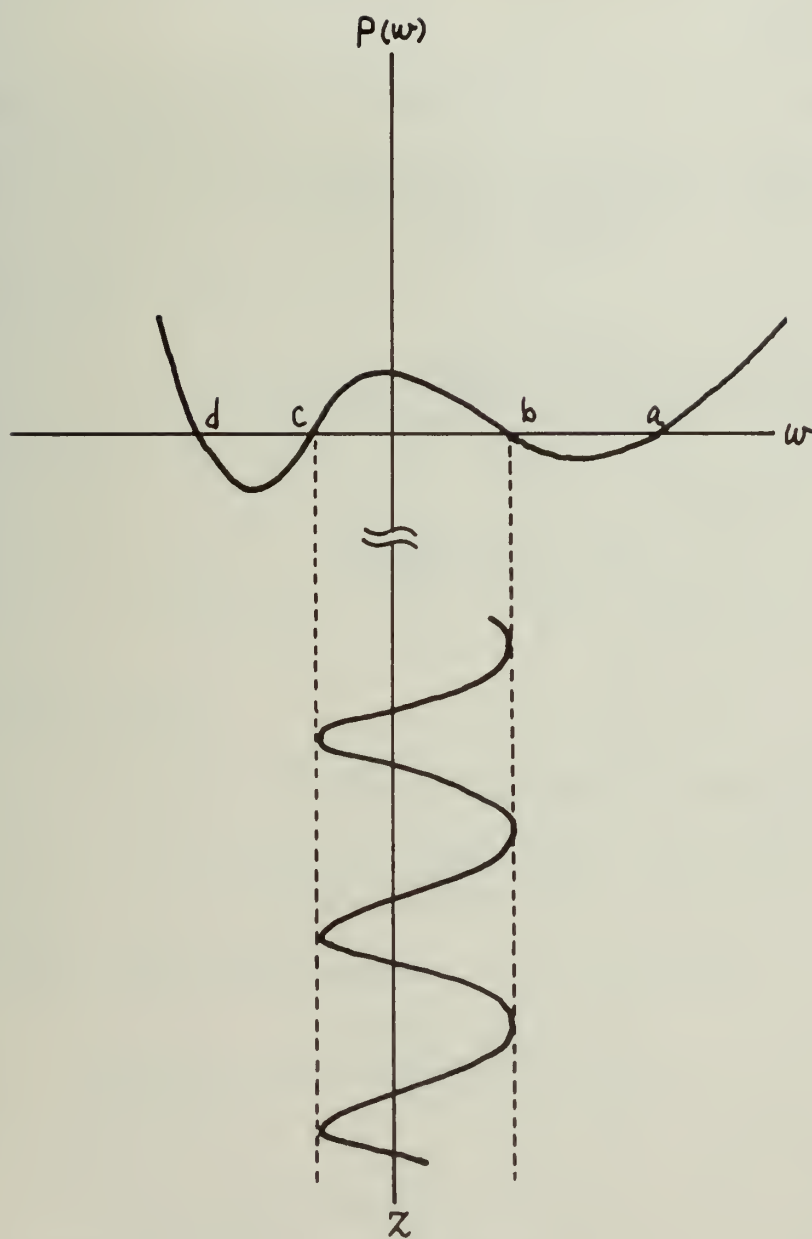


Fig. 3.10. Cubic nonlinearity ($\mu < 0$): periodic wave.

or

$$w_{II}(z) = \frac{b-a \left(\frac{b-c}{a-c}\right) \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)}{1 - \left(\frac{b-c}{a-c}\right) \operatorname{sn}^2 \left(\frac{\sqrt{(a-c)(b-d)}}{2} \rho z, k \right)}.$$

As is discussed in Appendix C, these two solutions differ from each other only by phase. That is, we can match w_I and w_{II} by shifting one of them by $2K/\rho\sqrt{(a-c)(b-d)}$.

Going back to the x, t coordinates, w_I and w_{II} are, respectively,

$$u_I(x-vt) = \frac{c-d \left(\frac{b-c}{b-d}\right) \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)}{1 - \left(\frac{b-c}{b-d}\right) \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)} \quad (3.37a)$$

and

$$u_{II}(x-vt) = \frac{b-a \left(\frac{b-c}{a-c}\right) \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)}{1 - \left(\frac{b-c}{a-c}\right) \operatorname{sn}^2 \left(\frac{2K}{\pi} (k_x x - \omega t), k \right)} \quad (3.37b)$$

where

$$k_x = \frac{C_o \pi}{4K} \sqrt{\frac{\mu(a-c)(b-d)}{6\epsilon}}$$

$$\omega = vk_x$$

$$K = k(k).$$

The velocity is given by (3.36a) and (3.36b):

$$\begin{aligned} v^2 &= C_o^2 \left[1 + \frac{\epsilon^2}{3|\mu|} - \frac{|\mu|}{12} (a^2 + b^2 + c^2 + d^2) \right] \\ &= C_o^2 \left[1 + \frac{\epsilon}{3} (a+b+c) - \frac{|\mu|}{12} \{ (a-b)^2 + (b-c)^2 + (c-a)^2 \} \right]. \end{aligned} \quad (3.38)$$

We can see that the velocity is always less than $C_o^2 (1 + \frac{\epsilon^2}{3|\mu|})$. In particular the velocity is less than C_o if $\epsilon = 0$. We should note the periodic wave solution is always unstable for a large enough amplitude when μ is negative. Therefore the only amplitude that yields the right hand side of (3.38) positive is admissible.

Periodic Wave around the Natural Length

Since we consider a symmetric wave around $w=0$, we put $b=-c > 0$, hence $a=-d > 0$ (Fig. 3.11). We also assume that $\epsilon=0$ for the sake of simplicity. Therefore

$$k^2 = \frac{4ab}{(a+b)^2}$$

$$k_x = \frac{C_o \pi}{4K} \sqrt{\frac{\mu}{6\kappa}} (a+b)$$

and

$$v^2 = C_o^2 \left[1 - \frac{\mu}{6} \{ (a+b)^2 + 2b^2 - 2ab \} \right] = C_o^2 \left[1 - \frac{\mu}{6} \left\{ \left(1 - \frac{k^2}{2}\right) (a^2 + b^2) + 2b^2 \right\} \right] < C_o^2.$$

From the above three equations, we have

$$\begin{aligned} v^2 &= C_o^2 \left[1 - \frac{\mu}{6} \left(1 - \frac{k^2}{2}\right) \left(\frac{4K}{C_o \pi}\right)^2 \frac{6\kappa}{\mu} k_x^2 - \frac{\mu}{3} b^2 \right] \\ &= C_o^2 \left(1 - \frac{\mu}{3} b^2\right) - \kappa \left(\frac{4K}{\pi}\right)^2 \left(1 - \frac{k^2}{2}\right) k_x^2, \end{aligned} \quad (3.39)$$

or

$$\omega^2 = C_o^2 k_x^2 - \frac{\mu C_o^2}{3} - \kappa \left(\frac{4K}{\pi}\right)^2 \left(1 - \frac{k^2}{2}\right) k_x^4. \quad (3.40)$$

Solitary Wave

If either a approaches to b in (3.37a) or d approaches to c in (3.37b), we have the solitary wave solution on the positive (rarefactive) background or on the negative (compressive) background, respectively. Since $\text{sn}^2 \rightarrow \tanh^2$, these solutions are, respectively,

$$u(x-vt) = \frac{c-d \left(\frac{b-c}{b-d}\right) \tanh^2(\alpha x - \beta t)}{1 - \left(\frac{b-c}{b-d}\right) \tanh^2(\alpha x - \beta t)} \quad (3.41a)$$

and

$$u(x-vt) = \frac{b-a \left(\frac{b-c}{a-c}\right) \tanh^2(\alpha x - \beta t)}{1 - \left(\frac{b-c}{a-c}\right) \tanh^2(\alpha x - \beta t)} \quad (3.41b)$$

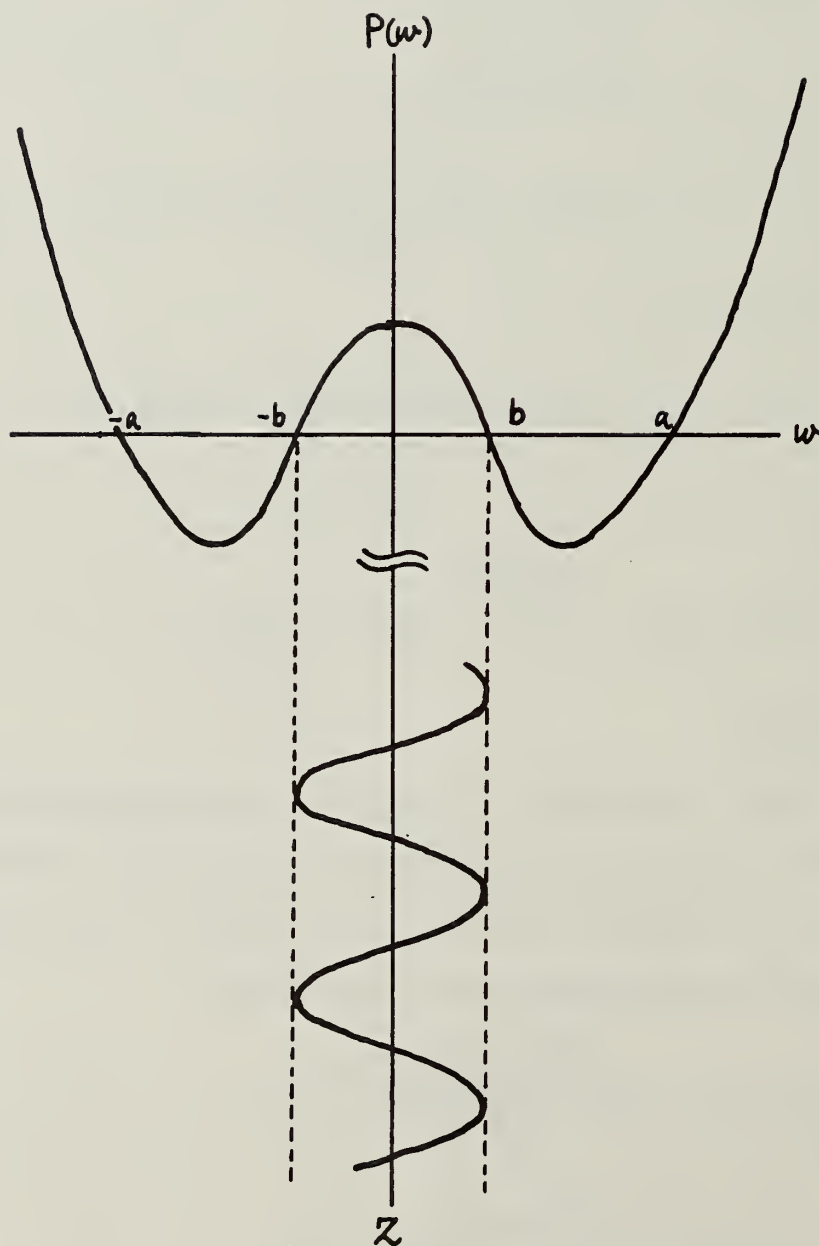


Fig. 3.11. Cubic nonlinearity ($\mu < 0$): periodic wave (symmetric).

where

$$\alpha = \frac{\sqrt{(a-c)(b-d)}}{2} \quad \rho = \sqrt{\frac{\mu C_o^2 (b-c)(b-d)}{24\kappa}} \quad \text{for (3.41a)}$$

$$= \sqrt{\frac{(a-c)(b-c)\mu C_o^2}{24\kappa}} \quad \text{for (3.41b)}$$

$$\beta = v \cdot \gamma$$

and

$$v^2 = C_o^2 \left(1 - \frac{\mu}{6} (b-c)^2\right) \quad \text{for both cases}$$

$$= C_o^2 \left(1 - \frac{\mu}{6} A^2\right) .$$

Note that there is no solitary wave solution on zero background: if $a=b$ were 0, it would give $a+b+c+d = c+d=0$. But this is contradictory to $d < c < 0$. On the other hand, if $c=d$ were 0, it would give $a+b=0$ which contradicts the condition $a > b > 0$. Hence the above proposition is proved. This corresponds to the fact that $\frac{df(x)}{dx}$, where $f(x)$ is the force function, takes the maximum

Extra Solution

There is also an extra solution for $\mu < 0$. But this solution is quite different from the algebraic solitary wave for $\mu > 0$: it requires the positive background on one side of the lattice and the negative background on the other. Since we are not interested in this solution, we will give only a brief description. We assume that $P(w)$ has two double roots a and $-a$ (Fig. 3.12). The equation is

$$\begin{aligned} \left(\frac{dw}{dz}\right)^2 &= \mu^2 (w+a)^2 (a-w)^2 \\ &= \mu^2 (a^2 - w^2)^2, \end{aligned}$$

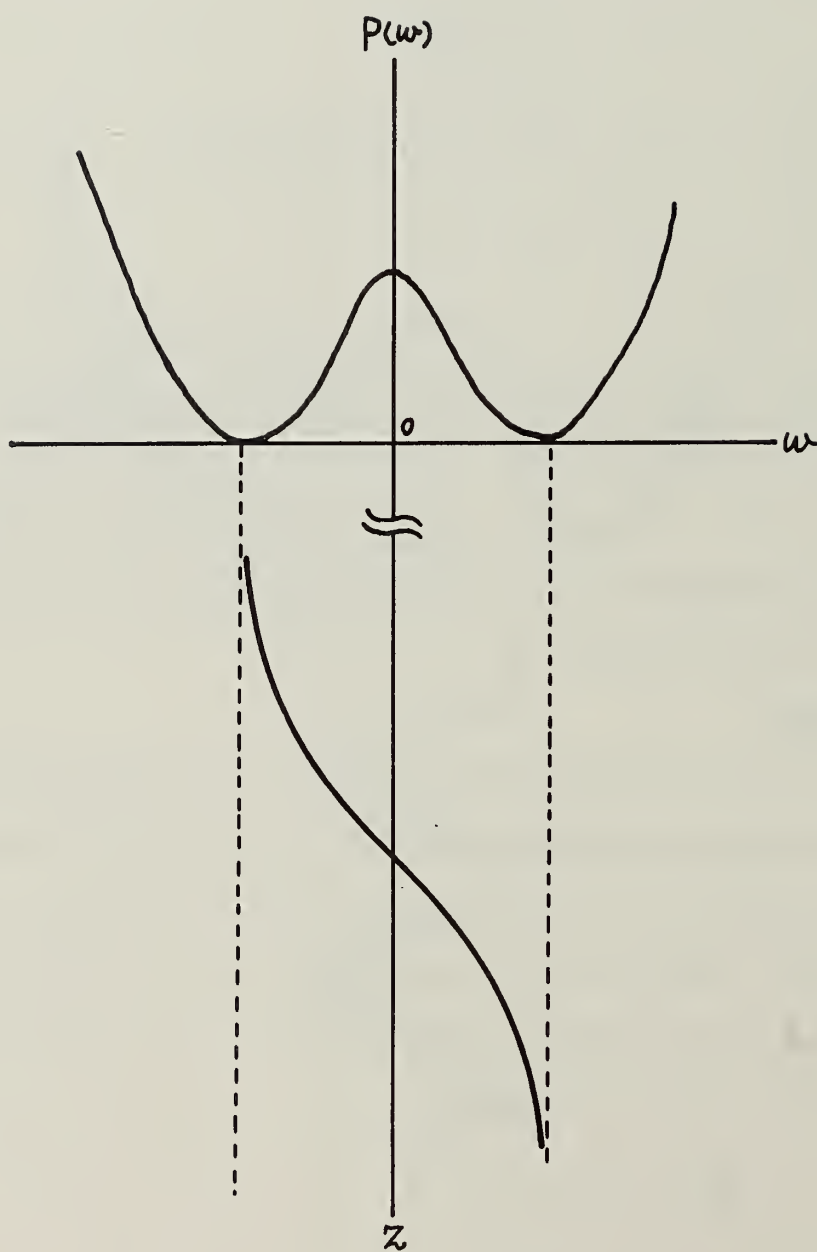


Fig. 3.12. Cubic nonlinearity ($\mu < 0$): non-solitary wave solution.

the solution which is

$$w = a \cdot \tanh(az)$$

$$v^2 = c_o^2 \left(1 - \frac{\mu a^2}{3n} \right) .$$

Table 3.1 summarizes all the solutions discussed in §3.2 and §3.3.

3.4 Piecewise Linear Approximation and Explanation of the Existence of Solitary Waves

So far we have treated the polynomial type force functions extensively. We have made use of the special properties of the elliptic functions in deriving the solutions. Some of the common characteristics of the solutions are:

- (1) the periodic solution can be either supersonic or subsonic depending on the wave form;
- (2) the solitary wave solution is a special case of the periodic solution;
- (3) the solitary wave is always formed in such a way that the interaction force becomes stiffer as the displacement increases;
- (4) the propagation velocity of the solitary wave is always higher than the ambient sound velocity;
- (5) the wave form of the solitary wave may be approximated by the exponential function in the region where the displacement is small.

On the other hand we learned in Chapter 2 that the harmonic lattice has the exponential solutions as well as the sinusoidal solutions. This fact together with (3) and (5) suggests the force described by two linear functions as a simple model:

Table 3.1
Summary of all the possible solutions in §3.2 and §3.3

	force	periodic solution	solitary wave	extra solution
QUADRATIC	$\epsilon \neq 0$ $\xi > 0$ 			
	$\mu = 0$ $\xi < 0$ 			
CUBIC	$\mu \neq 0$ $\mu > 0$ 			
	$\epsilon = 0$ $\mu < 0$ 			

$$\begin{aligned}
 f(x) &= x & x > b \\
 &= (1+\Delta)x - \Delta b & x < b . \quad (\text{Fig. 3.13})
 \end{aligned}$$

The equation which corresponds to (3.5) in each region of u is the following:

$$\begin{aligned}
 \ddot{u} &= C_o^2 \ddot{u} + \kappa u''' & u > b \\
 \ddot{u} &= C_o^2 (1+\Delta) u'' + \kappa u''' & u < b .
 \end{aligned}$$

We assume that the solution $u(x-vt)$, its first derivative and its second derivative are continuous at $u=b$. Putting $w(z) = b-u(x-vt)$ and integrating the equations for $w(z)$ twice with respect to z yield

$$\kappa w'' = (v^2 - C_o^2)w + D_1 z + E_1 \quad (w < 0) \quad (3.42a)$$

$$\kappa w'' = [v^2 - C_o^2 (1+\Delta)]w + D_2 z + E_2 \quad (w > 0) \quad (3.42b)$$

where D_1 , E_1 , D_2 , and E_2 are the integration constants. As we discussed in §3.1, we can put $D_1 = D_2 = 0$. From the condition that w'' is continuous at $w=0$, we have $E_1 = E_2 = E$. Multiplying the both hand sides of (3.42a) and (3.42b) by w' and integrating with respect to z yield

$$\frac{\kappa}{2} w'^2 = (v^2 - C_o^2) \frac{w^2}{2} + Ew + F_1 \quad w < 0 \quad (3.43a)$$

$$\frac{\kappa}{2} w'^2 = [v^2 - C_o^2 (1+\Delta)] \frac{w^2}{2} + Ew + F_2 \quad w > 0 \quad (3.43b)$$

where F_1 and F_2 are the integration constants. From the condition that w' is continuous at $w=0$, $F_1 = F_2 = F$. Dividing the both hand sides of the above equations by $\frac{\kappa}{2}$ yields

$$w'^2 = \frac{v^2 - C_o^2}{\kappa} w^2 + \frac{2E}{\kappa} w + \frac{2F}{\kappa} = P_1(w) \quad w < 0 \quad (\text{region I}) \quad (3.44a)$$

$$w'^2 = \frac{v^2 - C_o^2 (1+\Delta)}{\kappa} w^2 + \frac{2E}{\kappa} w + \frac{2F}{\kappa} = P_2(w) \quad w > 0 \quad (\text{region II}) . \quad (3.44b)$$

Obviously, $P_2(w) = P_1(w) - \frac{C_o^2 \Delta}{2\kappa} w^2$.

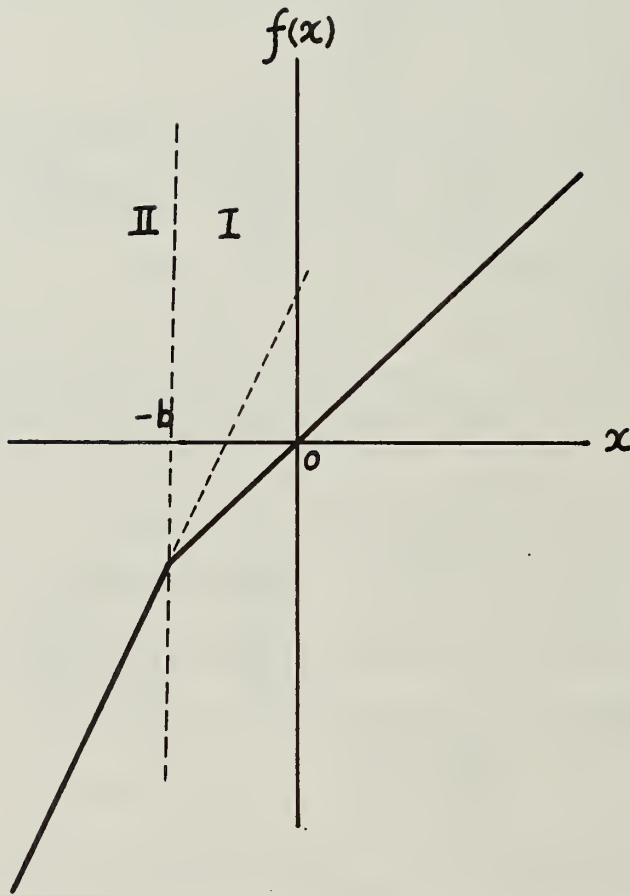


Fig. 3.13. A typical piecewise linear force function (one break point).

The solutions of the differential equation of the forms given in (3.44) are known to be either the sinusoidal functions or the hyperbolic functions, the exponential function being included in the latter as a special case. More explicitly, if the quadratic polynomial $P_1(w)$ or $P_2(w)$ has the positive leading coefficient, the solution is $\pm \cosh$, $\sinh$ or $\exp$ depending on whether the discriminant of the polynomial is positive, negative or zero, respectively. On the other hand, if the leading coefficient is negative, the solution is the sinusoidal function, provided that the discriminant is positive; otherwise there is no real solution. In solving (3.44) we can select one of the above mentioned functions in each region, depending on the leading coefficient and the discriminant of $P_1(w)$ or $P_2(w)$, then connect them in such a way that the derivatives of the selected functions match up to the second order at $w=0$. There are two different cases of our interest.

3.4.1 $v^2 < C_0^2$ (Subsonic Waves)

Both $P_1(w)$ and $P_2(w)$ have the negative leading coefficients. Obviously, we have the periodic solution in $[w_1, w_2]$ where w_2 is the smaller zero of $P_2(w)$ and w_1 is the larger zero of $P_1(w)$. (Fig. 3.14.) The solution may be obtained by connecting two sinusoidal waves at $w=0$. The resulting wave is not symmetric with respect to the z -axis due to the difference between $P_1(w)$ and $P_2(w)$. In order to maintain the wave form as the composite wave propagates, the phase velocity of the wave in each region must be the same. This is best explained graphically by using the dispersion curves (Fig. 3.15). Since the force function is steeper in region II, the dispersion curve for this region is always located above that for region I. For a given phase velocity v_p , we draw a straight line in the ω - k_x plane, which

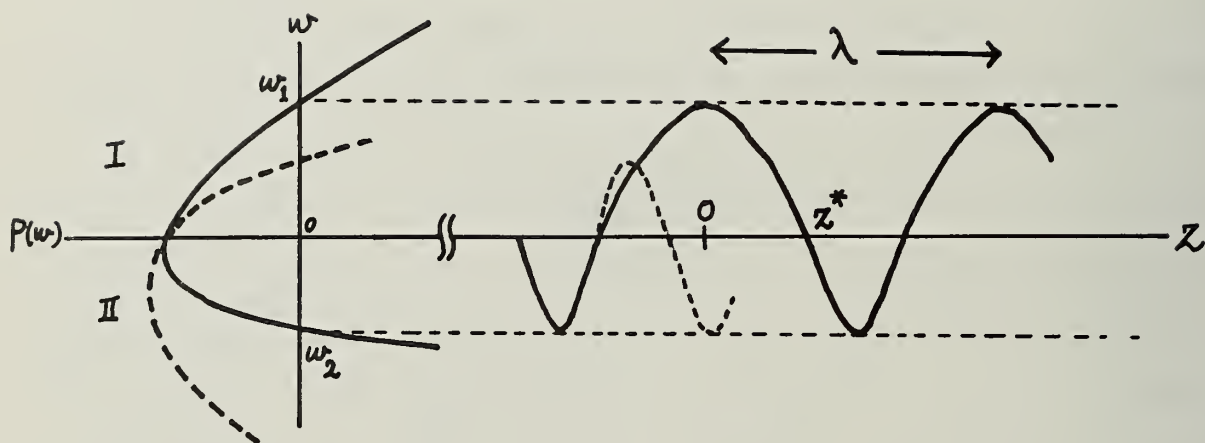


Fig. 3.14. Subsonic wave in piecewise linear lattice.

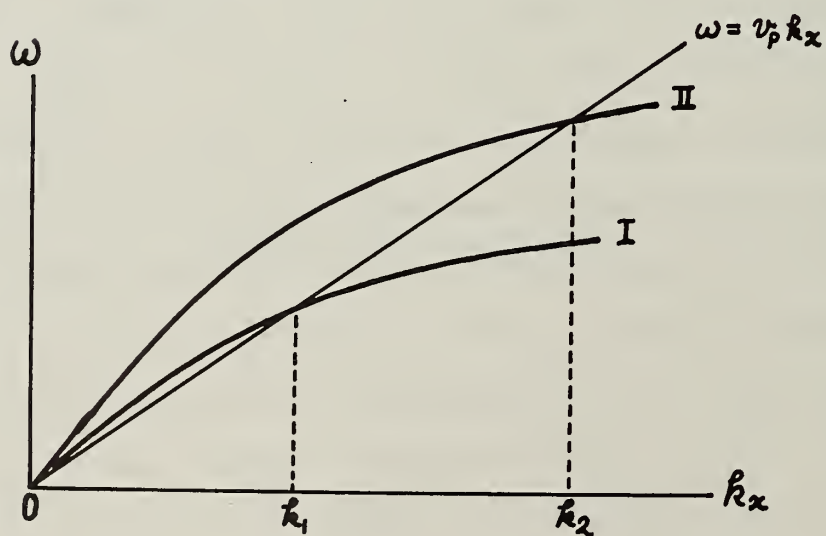


Fig. 3.15. Dispersion relation for subsonic waves.

crosses two dispersion curves at k_1 and k_2 . This is possible for a suitably chosen v_p . Then we put the solution in region I as

$$w_I(z) = A_1 \cos(k_1 z) + B_1 \quad (3.45a)$$

and the solution in region II as

$$w_{II}(z) = +A_2 \cos(k_2 z + \phi) + B_2. \quad (3.45b)$$

We have the following six equations to determine A_1 , B_1 , P , A_2 , B_2 , z^* from (where $w_I(z^*) = w_{II}(z^*) = 0$):

$$A_1 + B_1 = w_1 > 0 \quad (3.46a)$$

$$A_1 \cos(k_1 z^*) + B_1 = 0 \quad (3.46b)$$

$$B_2 - A_2 = w_2 < 0 \quad (3.46c)$$

$$A_2 \cos(k_2 z^* + \phi) + B_2 = 0 \quad (3.46d)$$

$$A_1 k_1 \sin(k_1 z^*) = A_2 k_2 \sin(k_2 z^* + \phi) \quad (3.46e)$$

$$A_1 k_1^2 \cos(k_1 z^*) = A_2 k_2^2 \cos(k_2 z^* + \phi). \quad (3.46f)$$

From these equations we can eliminate all but A_1 and A_2 , resulting in the following two equations, each representing a hyperbola:

$$\frac{k_1^2}{w_2^2 (k_2^2 - k_1^2)} A_1^2 - \frac{k_2^4}{k_1^2 w_2^2 (k_2^2 - k_1^2)} \left[A_2 + \frac{w_2 (k_2^2 - k_1^2)}{k_2^2} \right]^2 = 1 \quad (3.47a)$$

$$\frac{k_1^4}{k_2^2 w_1^2 (k_2^2 - k_1^2)} \left[A_1 + \frac{w_1 (k_2^2 - k_1^2)}{k_1^2} \right]^2 - \frac{k_2^2}{w_1^2 (k_2^2 - k_1^2)} A_2^2 = 1. \quad (3.47b)$$

We can solve (3.47) for A_1 and A_2 graphically (Fig. 3.16).

Since there is only one intersection of the two graphs, A_1 and A_2 are determined uniquely for the given set of k_1 , k_2 , w_1 and w_2 . We can obtain all other unknowns in a straightforward manner from (3.46). By

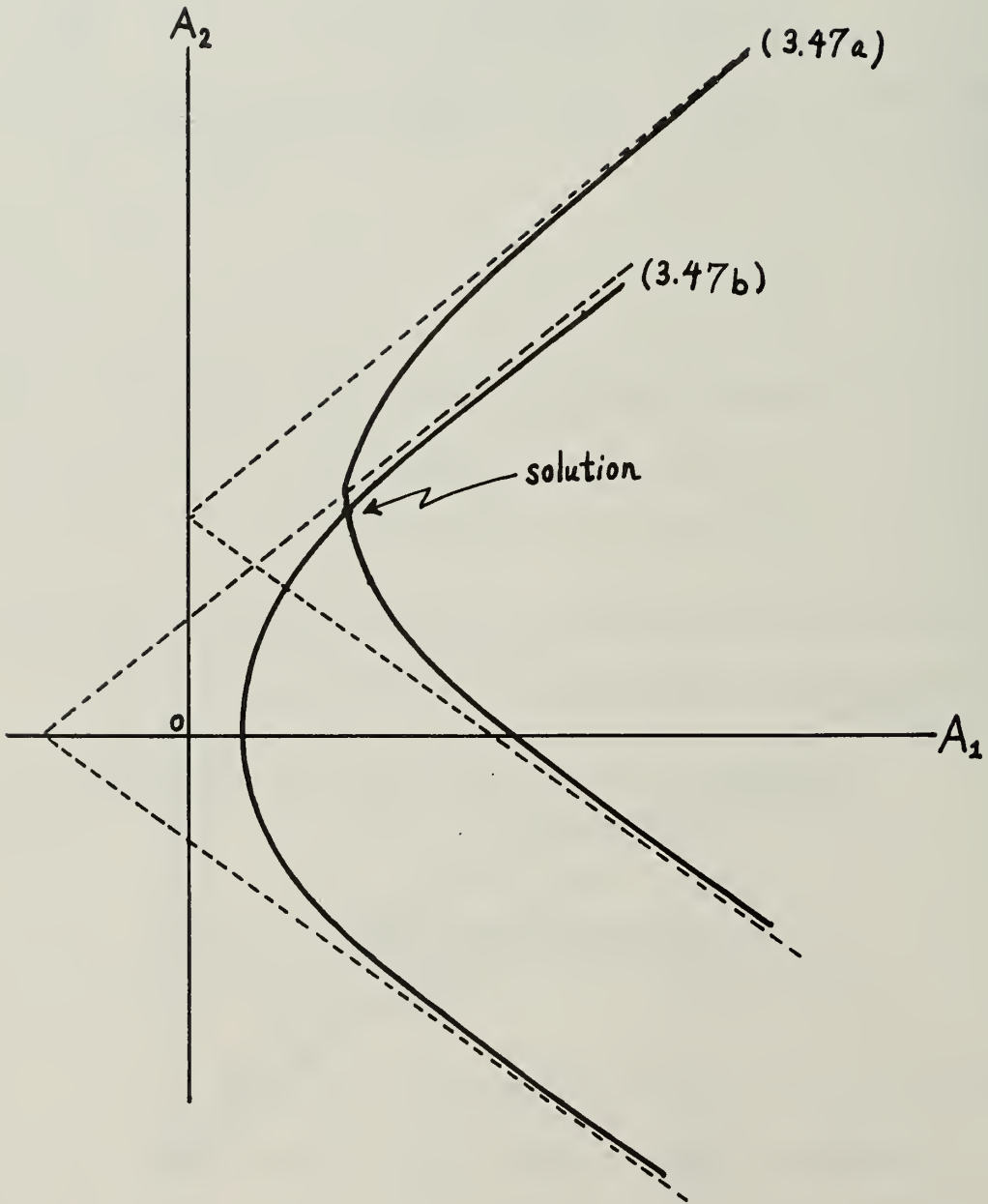


Fig. 3.16. Graphical solution of (3.47).

changing v_p , it is possible to obtain the relations among such quantities as the amplitude ($w_1 + w_2$), the wave number and frequency, but we will not go into the detailed discussion, since we are interested in showing the existence of the solutions similar to those in §3.2 and the feasibility of the piecewise linear model rather than the numerical calculation.

$$3.4.2 \quad C_o^2 < v^2 < C_o^2(1+\Delta) \quad (\text{Supersonic Wave})$$

In this case $P_1(w)$ has the positive leading coefficient, whereas $P_2(w)$ has the negative leading coefficient. Both the periodic wave and the solitary wave solutions exist depending on the discriminant of $P_1(w)$.

Periodic Wave

The periodic wave is obtained by choosing the cosh function in the region I and the cos function in the region II, then connecting them together (Fig. 3.17). The dispersion relations are

$$\omega^2 = C_o^2 k_x^2 + \mu k_x^4 \quad (\text{region I})$$

$$\omega^2 = C_o^2(1+\Delta)k_x^2 - \mu k_x^4 \quad (\text{region II}) .$$

They are also shown in Fig. 3.18.

Solitary Wave

As the discriminant of $P_1(w)$ vanishes, the periodic wave reduces to the solitary wave (Fig. 3.19). In such limit the wave consists of two exponentially decaying curves and a part of the sinusoidal curve, since $\cosh(z)$ reduces to $\exp(z)$ or $\exp(-z)$. The dispersion curves are given in Fig. 3.18.

It is obvious from the foregoing discussion why the crest of the solitary wave must be formed in the region II, where the force function is steeper: only in such case can the sinusoidal part of the wave propagate

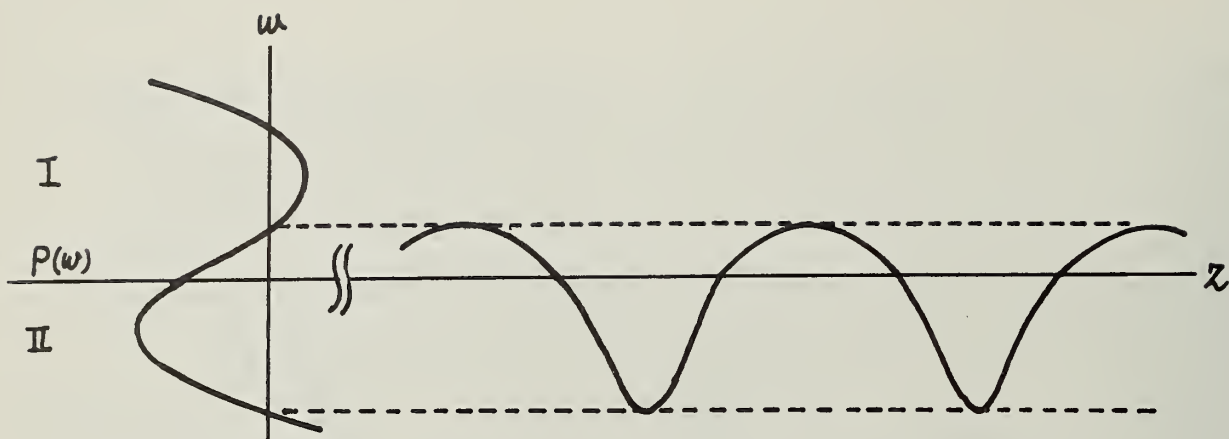


Fig. 3.17. Supersonic wave (periodic) in piecewise linear lattice.

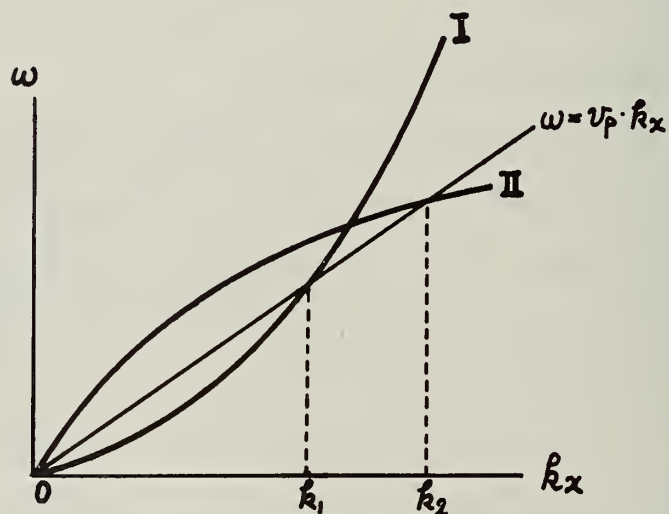


Fig. 3.18. Dispersion relation for supersonic wave.

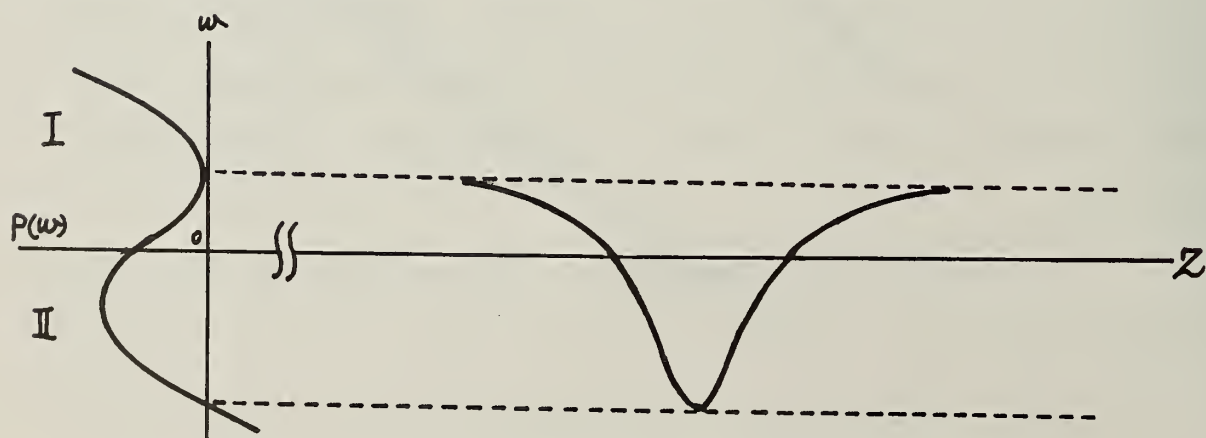


Fig. 3.19. Solitary wave in piecewise linear lattice.

as fast as the exponential part. Also note that the combination of the exponential function and the sinusoidal function is possible only in the supersonic case.

3.4.3 Summary

We have shown that all the features of the waves in the anharmonic lattice (in continuum approximation) listed at the beginning of this section can be elementary explained by the piecewise linear force model. We believe that this approach is quite feasible.

As is evident from Fig. 3.14, Fig. 3.17 and Fig. 3.19, approximating a quadratic force function by two linear functions is equivalent to approximating a cubic polynomial by two parabolas in the $P(w)$ - w plane. We can obtain a better approximation to a given force function by extending this approach to include more break points. For example, a cubic force function in §3.3 is essentially approximated by three linear functions (Fig. 3.20). It is clear that the compressive solitary wave and the rarefactive solitary wave exist as well as the periodic wave for such function. The only exception is the algebraic solitary wave, since it stems from the multiple zero of order three or more of the polynomial $P(w)$ in the equation

$$\left(\frac{dw}{dz}\right)^2 = P(w).$$

The analytic approach in §3.2 and §3.3 will be very difficult for the higher order polynomial $P(w)$, since we are quite dependent on the special properties of the Jacobian elliptic functions. One of the advantages of our approach in this section is that we can obtain the approximate solutions for the higher order polynomials as well, since we are dealing with elementary functions.

We will give some of the numerical examples in §5.5. We will consider the hardsphere and harmonic force in Chapter 5, which is an extreme case of our approximation here.

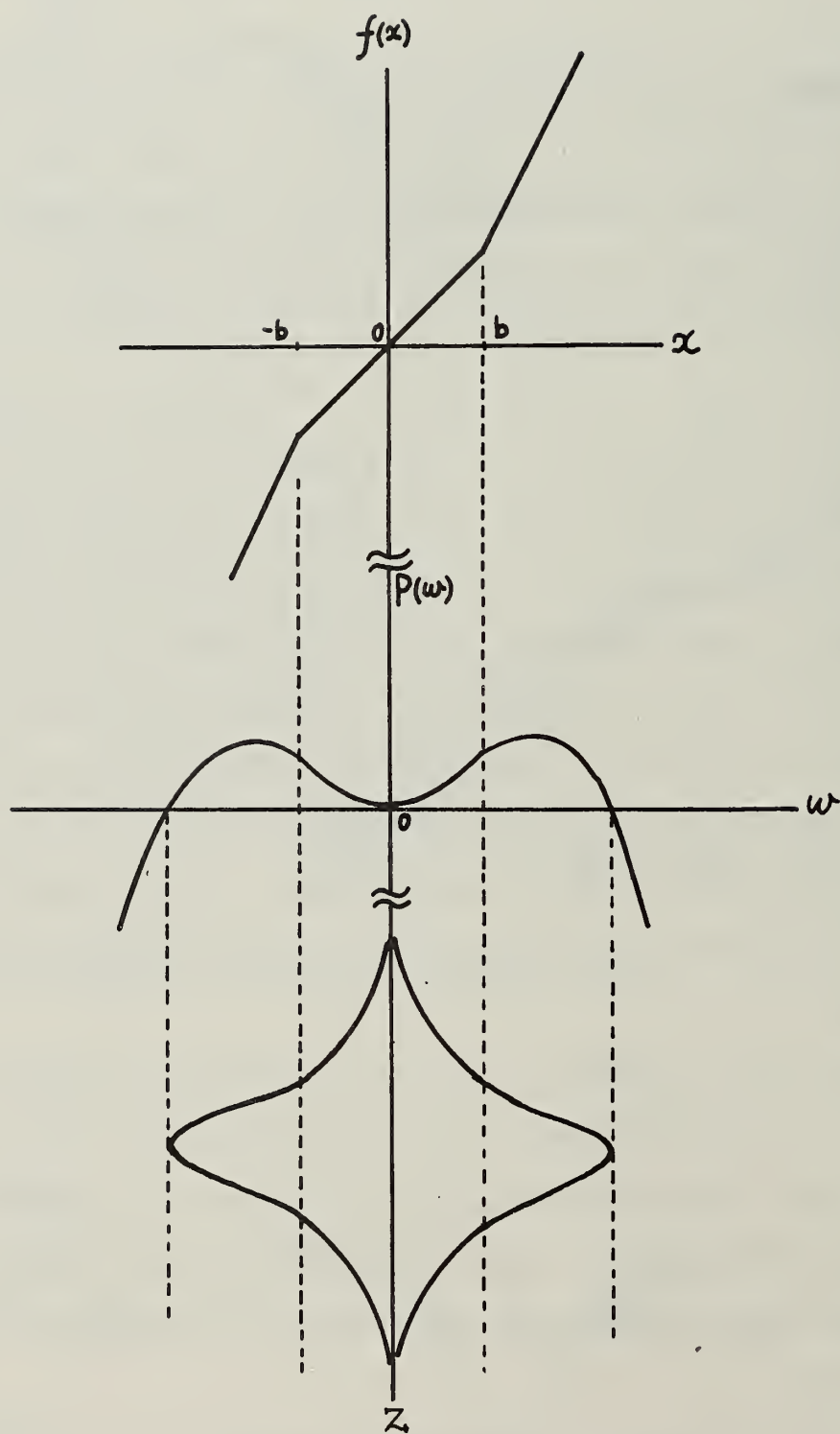


Fig. 3.20. Solitary waves in piecewise linear lattice (two break points).

3.5 Toda's Solution for the Exponential Lattice

The solutions obtained in the continuum approximation are valid only when the wave form varies gradually. The only exact solutions known for the anharmonic lattice are those obtained by Toda.^{(10), (11)} In this section we briefly summarize the results obtained by Toda and compare them with the solutions obtained in §3.2.

Toda considered the interaction force which is defined as

$$f(x) = \frac{1}{b}(1 - \exp(-bx)) \quad (3.48)$$

where b is a parameter which determines the degree of nonlinearity. If we consider the lattice with an infinite number of atom, the first term in (3.48) vanishes; Toda's force function is essentially the repulsive force. $f(x)$ may be expanded in the Taylor series

$$f(x) = x - \frac{b}{2} x^2 + \frac{b^2}{6} x^3 - \dots \quad (3.49)$$

Hence, exponential force may be approximated by the quadratic nonlinearity if x is sufficiently small.

The exact equation of motion is

$$\frac{d^2 u_n}{dt^2} = \frac{1}{b}(2e^{-bu_n} - e^{-bu_{n+1}} - e^{-bu_{n-1}}), \quad (3.50)$$

where $u_n = y_{n+1} - y_n$ is the difference of the displacement of two neighboring atoms.

Toda found two particular solutions of different types, one being the solitary wave and the other being the periodic wave. The solitary wave solution is given as

$$u_n = -\frac{1}{b} \log(1 + \beta^2 \operatorname{sech}^2(\alpha n + \beta t)) \quad (3.51)$$

$$\text{where } \beta = \sinh \alpha. \quad (3.52)$$

Note that the relation (3.52) is identical to the one given for the unbounded solution of the harmonic lattices (§2.1). This is not a coincidence. Toda's solution (3.51) approaches to the exponential function as $\alpha n \mp \beta t \rightarrow \infty$. That is, the outskirts of the solitary wave behave like the wave in the harmonic lattices, for which $\beta = \sinh \alpha$ holds exactly. Since Toda's solution is a traveling wave, the same relation between α and β should hold all over the wave. Hence, (3.52) seems to hold quite generally for the solitary waves in the anharmonic lattice.

If we expand (3.51) and (3.52) in the Taylor series, the first order terms are

$$u_n = -\beta^2 \operatorname{sech}^2(\alpha n \mp \beta t) \quad (\beta^2 \ll 1)$$

and

$$\beta^2 = \left(\alpha \mp \frac{\alpha^3}{6}\right)^2 \approx \alpha^2 \left(1 \mp \frac{\beta^2}{3}\right).$$

From the latter equation the velocity yields

$$v^2 = \frac{\beta^2}{\alpha^2} = 1 \mp \frac{\beta^2}{3},$$

which matches (3.13) if we put $c_0^2 = 1$ and $\varepsilon = 1$.

As for the periodic wave, the exact solution is

$$u_n = -\log \left[1 + \left(\frac{2K\omega}{\pi} \right)^2 \left\{ \operatorname{dn}^2 \left(\frac{2K}{\pi} (k_x n \mp \omega t) \right) - \frac{E}{K} \right\} \right] \quad (3.53)$$

where ω and k_x are related in the following way:

$$\frac{2K\omega}{\pi} = \frac{\operatorname{sn} \left(\frac{2K}{\pi} k_x \right)}{\sqrt{1 + \left(\frac{E}{K} - 1 \right) \operatorname{sn}^2 \left(\frac{2K}{\pi} k_x \right)}}. \quad (3.54)$$

The relation between the phase velocity and the wave number is obtained from (3.54) and is shown in Fig. 3.21. The curves are very close

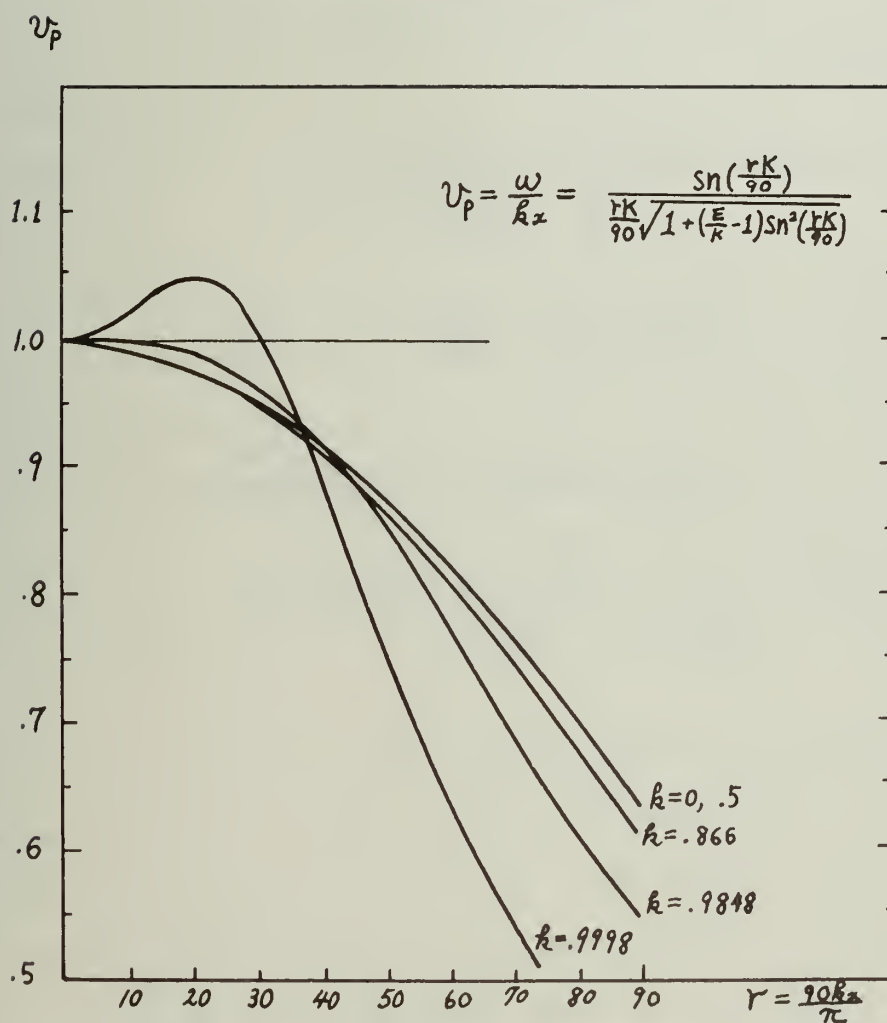


Fig. 3.21. Phase velocity vs wave number relation for Toda's lattice.

to that for the harmonic lattice if k is small. As k increases the velocity starts to take values greater than C_0 for the lower wave numbers. Clearly the periodic wave for Toda's exponential lattice can be either supersonic or subsonic. The Taylor expansion is valid when $k^2 \left(\frac{2K\omega}{\pi}\right)^2 \ll 1$ since the amplitude of $(\text{dn}^2 - \frac{E}{K})$ is k^2 . Therefore either k or ω should be small compared with 1. Then the first order approximation is

$$u_n = -\left(\frac{2K\omega}{\pi}\right)^2 \left[\text{dn}^2 \left\{ \frac{2K}{\pi} (\omega t + k_x n) \right\} - \frac{E}{K} \right]. \quad (3.55)$$

The dispersion relation yields

$$\begin{aligned} \left(\frac{2K\omega}{\pi}\right)^2 &\approx \frac{\left(\frac{2K}{\pi} k_x\right)^2 - \frac{1+k^2}{3} \left(\frac{2K}{\pi} k_x\right)^4}{1 + \left(\frac{E}{K} - 1\right) \left(\frac{2K}{\pi} k_x\right)^2} \\ &\approx \left(\frac{2K}{\pi} k_x\right)^2 - \left(\frac{1+k^2}{3} + \frac{E}{K} - 1\right) \left(\frac{2Kk_x}{\pi}\right)^4 \\ &= \left(\frac{2K}{\pi} k_x\right)^2 + \frac{1}{3} (2 - k^2 - \frac{3E}{K}) \left(\frac{2Kk_x}{\pi}\right)^4 \end{aligned} \quad (3.56)$$

where we have made use of the following approximation:

$$\text{sn}(x, k) \approx x - \frac{1+k^2}{6} x^3 \quad (k, x \ll 1).$$

We can easily show that (3.56) matches (3.11) if we put $C_0 = 1$, $\kappa = \frac{1}{12}$.

It is expected that the Taylor expansion of (3.53) up to the second order matches the solution for the cubic nonlinearity (§3.3), provided that the latter solution (which is in the form of the rational function) is also expanded in the Taylor series and the terms with the order of sech^6 and higher are truncated. Detailed calculation will not be made here.

Toda also discovered the two solitary wave solution for the exponential lattice. He could show that there is a phase shift after the

two such waves collide each other. The phase relation is such that if two waves make a head-on collision the phase shift is positive for both waves, whereas if one wave takes over the other, the phase shift for the faster wave is positive and the phase shift for the slower one is negative. The important thing is that these waves preserve their identity even after the collision, unlike the conventional shock waves in the dissipative medium.

Recently Wadati and Toda showed that both the original equation of motion (3.46) and its continuum approximation (3.5) with $\mu=0$ give exactly the same phase shift for the two wave collision problem.⁽³²⁾ Therefore, we can expect that the continuum approximation gives quite good quantitative results as well as qualitative results.

Zabusky discussed in his recent report that a travelling sine wave in the anharmonic lattice breaks into many small solitary waves of different amplitudes and velocities ("L Soliton"). Since Zabusky chose the periodic boundary condition, we can expect that these small waves are actually the superposition of the periodic waves of different amplitudes and wave numbers, each of which are similar to Toda's periodic solutions.⁽³³⁾

CHAPTER 4. NUMERICAL METHODS AND RELATED TOPICS

As we introduced in §1.2, our model consists of two essential parts: the crystal lattice described by a set of ordinary differential equations and the heat reservoirs described by random sampling of the velocities. We need only the former part to investigate the transmission properties of the lattice (deterministic problem).

As for the lattice we have chosen the free boundary conditions on both ends, thus obtaining the following equations:

$$\begin{aligned} \frac{d^2 y_1}{dt^2} &= f(y_2 - y_1) && \text{(left end)} \\ \frac{d^2 y_n}{dt^2} &= f(y_{n+1} - y_n) - f(y_n - y_{n-1}) && (n=2 \sim N-1) \\ \frac{d^2 y_N}{dt^2} &= -f(y_N - y_{N-1}) && \text{(right end)} \end{aligned} \quad (4.1)$$

where y_n is the displacement of the n^{th} atom from its equilibrium position and f is given as

$$f(x) = x + \alpha x^2 + \beta x^3. \quad (4.2)$$

We can also write (4.1) in a vector form:

$$\frac{d^2}{dt^2} \vec{y} = \vec{F}(\vec{y})$$

where

$$\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \quad \vec{F} = \begin{bmatrix} f(y_2 - y_1) \\ f(y_3 - y_2) - f(y_2 - y_1) \\ \vdots \\ -f(y_N - y_{N-1}) \end{bmatrix}.$$

We also use the vector notation in this chapter when we mention the system of ordinary differential equations in general, in which case $\vec{F}$ may depend on $\vec{y}, t$ as well as on $\vec{y}$. If $\vec{F}$ depends on $\vec{y}$ only we call such system of equations "special equations" according to Henrici.⁽³⁴⁾ Throughout this chapter O.D.E. stands for the ordinary differential equations.

In §4.1 and §4.2 we discuss the numerical integration schemes. In §4.3 we discuss the heat reservoirs more in detail.

In §4.4 we discuss the computer system which we used and also the semi-interactive features of our programs. In §4.5 we show the typical structure of our programs by giving an example. (Also in Appendix D.)

4.1 Numerical Integration of the System of O.D.E.

Generally speaking, there are two different types of numerical integration schemes for the system of equations such as given in (4.1):

- (1) One step methods (Runge-Kutta type)
- (2) Multistep methods (Predictor-Corrector Methods).

As for the special equations, we can solve such equations directly without reducing them into a system of first order O.D.E. with $2N$ variables. Therefore we have four different types.

First, we compare the one step methods with the multistep methods.

- (1) The one step methods are self-starting, that is, we only have to specify the initial conditions. On the other hand, multistep methods require the information of several time steps before since in these methods we solve the finite difference equations. Especially in our problems, as will be clarified in §4.3, we have to restart the integration everytime the end atoms interact with the heat reservoirs. Therefore the multistep methods are very difficult to use.

(2) One step methods usually require more number of function evaluations per time step than the multistep methods do. A typical fourth order one step method requires four function evaluations per time step, whereas a comparable multistep method requires only two function evaluations per time step. In most cases this is the major obstacle against one step methods, since the function evaluation is the most time-consuming part. But in our present problems, as Waters extensively discussed,⁽³⁵⁾ the function which we deal with is the polynomial (cubic at most) and is very easily evaluated. Hence the one step methods are quite promising. Gear also mentioned this.⁽³⁶⁾ As for Toda's potential, however, this is not the case; if we need to do a long time computation with Toda's potential, the mixture of the multistep method (for the inner atoms) and the one step method (for those atoms which are near the boundary) will yield faster computation.*

(3) One step methods can be programmed very simple.

(4) Error bounds** for the multistep methods are more explicitly given than those for the one step methods. For the one step methods we have to evaluate the error by, for example, the step reduction technique.

From the above consideration we will solely discuss the one step methods for the integration of the equations (4.1).

*Remark given by C. W. Gear.

**There are two different types of errors in the numerical integration of O.D.E. One is the truncation error which stems from the approximation formula for integration. The other is the round-off error which stems from the finiteness of the length of the registers in the computer. Here, we are solely concerned with the former.

4.2 One Step Methods for the Special Equations

Usual technique to solve the second order O.D.E. is to reduce them to a system of first order O.D.E. by introducing extra variables $z_n = \dot{y}_n$.

There are quite a few integration schemes for the system of first order O.D.E. Most popular ones are Runge-Kutta's fourth order method (to be referred to as RKC4 in the following discussion) and its variations by Ralston and by Gill. These methods are listed in Table 4.1. Ralston's method was derived as a result of minimizing the truncation error of order h^4 , where h is the step size of integration.⁽³⁷⁾ This method gives the truncation error which is about 1/2 of that for RKC4. At the same time, however, the simpleness of the integration scheme is lost and more computation time results. Gill's method was derived from the viewpoint of reducing the size of temporary storage rather than an error consideration.⁽³⁸⁾ Blum later showed that the same reduction of temporary storage is possible for RKC4 too.⁽³⁴⁾ Therefore Gill's method is quite irrelevant nowadays. (Note that the simpleness of integration scheme is also lost in Gill's method.) Hence we can naturally select RKC4 as the most optimal one among the fourth order one step methods.* For a higher precision computation Waters⁽³⁵⁾ and Pasta et al.⁽¹⁸⁾ recommend Butcher's fifth order method. It is reported⁽¹⁸⁾ that the truncation error could be reduced as small as the round off error with a choice of $h = .01$. This is a "super accurate" example. Usually the truncation error is several orders larger than the roundoff error. We do not require such a high accuracy in our computation

* According to (39), p. 363, the Runge Kutta subroutines in most computer libraries still employ Gill's method. Probably this is just because the original (and the best!) method was derived in 1901, whereas Gill's method was derived in 1951, the latter giving an impression that it is quite improved.

Table 4.1

Classical Runge-Kutta (1901) ⁽³⁴⁾

$$\vec{y}_{n+1} = \vec{y}_n + \frac{h}{6}(\vec{K}_1 + 2\vec{K}_2 + 2\vec{K}_3 + \vec{K}_4)$$

$$\vec{K}_1 = \vec{F}(\vec{y}_n)$$

$$\vec{K}_2 = \vec{F}(\vec{y}_n + \frac{h}{2} \vec{K}_1)$$

$$\vec{K}_3 = \vec{F}(\vec{y}_n + \frac{h}{2} \vec{K}_2)$$

$$\vec{K}_4 = \vec{F}(\vec{y}_n + h\vec{K}_3)$$

Runge-Kutta-Ralston (1965) ⁽³⁷⁾

$$\begin{aligned} \vec{y}_{n+1} = \vec{y}_n + h(&.17476028\vec{K}_1 - .55148053 \vec{K}_2 \\ &+ 1.20553547\vec{K}_3 + .17118478\vec{K}_4) \end{aligned}$$

$$\vec{K}_1 = \vec{F}(\vec{y}_n)$$

$$\vec{K}_2 = \vec{F}(\vec{y}_n + .4h\vec{K}_1)$$

$$\vec{K}_3 = \vec{F}(\vec{y}_n + .29697760h\vec{K}_2 + .15875966h\vec{K}_2)$$

$$\vec{K}_4 = \vec{F}(\vec{y}_n + .21810038h\vec{K}_1 - 3.05096470h\vec{K}_2 + 3.83286432h\vec{K}_3)$$

Runge-Kutta-Gill (1951) ⁽³⁴⁾

$$\vec{y}_{n+1} = \vec{y}_n + \frac{h}{6}(\vec{K}_1 + (2+\sqrt{2})\vec{K}_2 + (2-\sqrt{2})\vec{K}_3 + \vec{K}_4)$$

$$\vec{K}_1 = \vec{F}(\vec{y}_n)$$

$$\vec{K}_2 = \vec{F}(\vec{y}_n + \frac{h}{2} \vec{K}_1)$$

$$\vec{K}_3 = \vec{F}(\vec{y}_n + \frac{h}{2}(-1+\sqrt{2})\vec{K}_1 + \frac{h}{2}(2-\sqrt{2})\vec{K}_2)$$

$$\vec{K}_4 = \vec{F}(\vec{y}_n - \frac{\sqrt{2}}{2} \vec{K}_2 + (1+\frac{\sqrt{2}}{2})\vec{K}_3)$$

Table 4.1 (continued)

Nystrom's method for the special equation (1925)⁽³⁴⁾

$$\vec{y}_{n+1} = \vec{y}_n + h \cdot \vec{y}'_n + \frac{h^2}{192}(23\vec{K}_1 + 75\vec{K}_2 - 27\vec{K}_3 + 25\vec{K}_4)$$

$$\vec{y}'_{n+1} = \vec{y}'_n + \frac{h}{192}(23\vec{K}_1 + 125\vec{K}_2 - 81\vec{K}_3 + 125\vec{K}_4)$$

$$\vec{K}_1 = \vec{F}(\vec{y}_n)$$

$$\vec{K}_2 = \vec{F}(\vec{y}_n + \frac{2}{5}h\vec{y}'_n + \frac{2}{25}h^2\vec{K}_1)$$

$$\vec{K}_3 = \vec{F}(\vec{y}_n + \frac{2}{3}h\vec{y}'_n + \frac{2}{9}h^2\vec{K}_1)$$

$$\vec{K}_4 = \vec{F}(\vec{y}_n + \frac{4}{5}h\vec{y}'_n + \frac{4}{25}h^2(\vec{K}_1 + \vec{K}_2))$$

Butcher's fifth order method (1964)⁽³⁵⁾

$$\vec{y}_{n+1} = \vec{y}_n + \frac{h}{90}(7\vec{K}_1 + 32\vec{K}_3 + 12\vec{K}_4 + 32\vec{K}_5 + 7\vec{K}_6)$$

$$\vec{K}_1 = \vec{F}(\vec{y}_n)$$

$$\vec{K}_2 = \vec{F}(\vec{y}_n - \frac{h}{2}\vec{K}_1)$$

$$\vec{K}_3 = \vec{F}(\vec{y}_n + \frac{h}{18}(5\vec{K}_1 - \vec{K}_2))$$

$$\vec{K}_4 = \vec{F}(\vec{y}_n + \frac{h}{4}(-3\vec{K}_1 + \vec{K}_2 + 4\vec{K}_3))$$

$$\vec{K}_5 = \vec{F}(\vec{y}_n + \frac{3h}{16}(\vec{K}_1 + \vec{K}_4))$$

$$\vec{K}_6 = \vec{F}(\vec{y}_n + \frac{h}{7}(-\vec{K}_2 + 12\vec{K}_3 - 12\vec{K}_4 + 8\vec{K}_5))$$

therefore a good compromise is the RKC4 or its equivalence in the sense of computational complexity (that is, the number of function evaluation per time step, the size of temporary storage, etc). Butcher's fifth order method is also given in Table 4.1.

An alternative approach is to integrate the second order O.D.E. without reducing it to the first order (direct method). Henrici discussed that the order of the truncation error for $\vec{y}$ do not match that for $\vec{y}$ in the general cases in which $\vec{F}$ depends on $\vec{y}$ as well as $\vec{y}$.⁽³⁴⁾ Therefore the direct methods are not recommended. But things are different for the special equations. Then, as Henrici pointed out,⁽³⁴⁾ not only the truncation error becomes the same order for $\vec{y}$ and $\vec{y}$ but also it is of the higher order error than the corresponding Runge Kutta methods. For example, two function evaluations yield a third order method, three function evaluations yield a fourth order method and four function evaluations yield a fifth order method. We are particularly interested in the fifth order method due to Nyström,⁽³⁴⁾ which is given in Table 4.1. RKC4 and the Nyström's fifth order method for the special equations (to be called NYS5) may be compared as follows:

(1) NYS5 yields higher order global error. That is, the total error at time t due to the truncation behaves approximately as $C_1 \cdot h^5$ for a given integration step h , where C_1 is a constant which depends on t and on other factors, and has to be evaluated for individual problems. As for RKC4 the total error at time t is approximately $C_2 \cdot h^4$. Hence if C_1 turns out to be comparable to C_2 for a given problem then NYS5 yields better results.

(2) The size of the temporary storage is smaller for NYS5. If we assume the nearest neighbor interactions only, NYS5 needs three temporary storage

Table 4.2
Comparison of NYS5 and RKC4

NYS5	RKC4
$\vec{K}_1 = \vec{F}(\vec{y}_n)$	$\vec{V}_1 = \vec{z}_n$ $\vec{K}_1 = \vec{F}(\vec{y}_n)$
$\vec{V}_2 = \vec{z}_n + \frac{h}{5}\vec{K}_1$	$\vec{V}_2 = \vec{z}_n + \frac{h}{2}\vec{K}_1$
$\vec{K}_2 = \vec{F}(\vec{y}_n + \frac{2h}{5}\vec{V}_2)$	$\vec{K}_2 = \vec{F}(\vec{y}_n + \frac{h}{2}\vec{V}_1)$
$\vec{V}_3 = \vec{z}_n + \frac{h}{3}\vec{K}_1$	$\vec{V}_3 = \vec{z}_n + \frac{h}{2}\vec{K}_2$
$\vec{K}_3 = \vec{F}(\vec{y}_n + \frac{2h}{3}\vec{V}_3)$	$\vec{K}_3 = \vec{F}(\vec{y}_n + \frac{h}{2}\vec{V}_2)$
$\vec{V}_4 = \vec{z}_n + \frac{h}{5}(\vec{K}_1 + \vec{K}_2)$	$\vec{V}_4 = \vec{z}_n + h\vec{K}_3$
$\vec{K}_4 = \vec{F}(\vec{y}_n + \frac{4h}{5}\vec{V}_4)$	$\vec{K}_4 = \vec{F}(\vec{y}_n + h\vec{V}_3)$
$\vec{z}_{n+1} = \vec{z}_n + \frac{h}{192}(23\vec{K}_1 + 125\vec{K}_2 - 81\vec{K}_3 + 125\vec{K}_4)$	$\vec{z}_{n+1} = \vec{z}_n + \frac{h}{6}(\vec{K}_1 + 2\vec{K}_2 + 2\vec{K}_3 + \vec{K}_4)$
$\vec{y}_{n+1} = \vec{y}_n + h\vec{z}_{n+1} - \frac{h^2}{192}(50\vec{K}_2 - 54\vec{K}_3 + 100\vec{K}_4)$	$\vec{y}_{n+1} = \vec{y}_n + \frac{h}{6}(\vec{V}_1 + 2\vec{V}_2 + 2\vec{V}_3 + \vec{V}_4)$
Note: V_2, V_3, V_4 are not necessary for actual computation. They are shown only to make comparison with RKC4. K_1, K_2, K_3 are the temporary vectors.	Note: $V_2, K_2, V_3, K_3, V_4, K_4$ are not necessary for actual computation since we can accumulate the sums $(K_1 + 2K_2 + 2K_3 + K_4)$ and $(V_1 + 2V_2 + 2V_3 + V_4)$ in K_1 and V_1 , respectively. On the other hand we need temporary vectors, one for $\vec{y}$ and the other for $\vec{z}$. Hence 4 temporary vectors are necessary.

vectors, whereas RKC4 needs four. In general they are four and eight, respectively. As a matter of fact, this difference is not so critical.

(3) The number of arithmetic operations (multiplication, addition) is almost the same for both methods, RKC4 being slightly superior to NYS5.

To compare the total error due to the truncation, we have run a test program with 50 atoms, $f = x - 10x^2 + 66.7x^3$. The initial velocities were given to two end atoms only. The error in the total energy at time 100 is given in Fig. 4.1 for h in $[.025, .2]$. As is clear from this figure, NYS5 was always superior to RKC4 in the given range of h . Any effect of the roundoff error was not observed even when $h = .025$. From this experiment we have decided to choose NYS5 over RKC4 for our computation.

4.3 Heat Reservoirs

As we introduced in §1.2, our heat reservoirs are defined dynamically, that is, they consist of gas molecules in thermal equilibrium. Take the left end, for example. At each step of integration (or at several steps as we will discuss later), the coordinate $y_1(t)$ and the velocity $\dot{y}_1(t)$ are examined to see if it will cross the boundary during the next time interval h . This is done by simple linear interpolation $y_1(t) + h \cdot \dot{y}_1(t)$. If this condition is met, the velocity is replaced by a new velocity, sampled at random from the left heat reservoir distribution of velocity,

$$P(v) = \frac{v}{T} \cdot e^{-\frac{v^2}{2T}}.$$
 A similar interaction occurs at the right end too. An interaction occurs only at the end of an integration step, hence no problem of the discontinuities; essentially we restart the integration with the new initial values at the end atoms everytime they (or one of them) hit the boundaries. See Gear.⁽³⁶⁾ Although we do not introduce any viscosity explicitly in this model, it essentially exists dynamically at the boundaries.

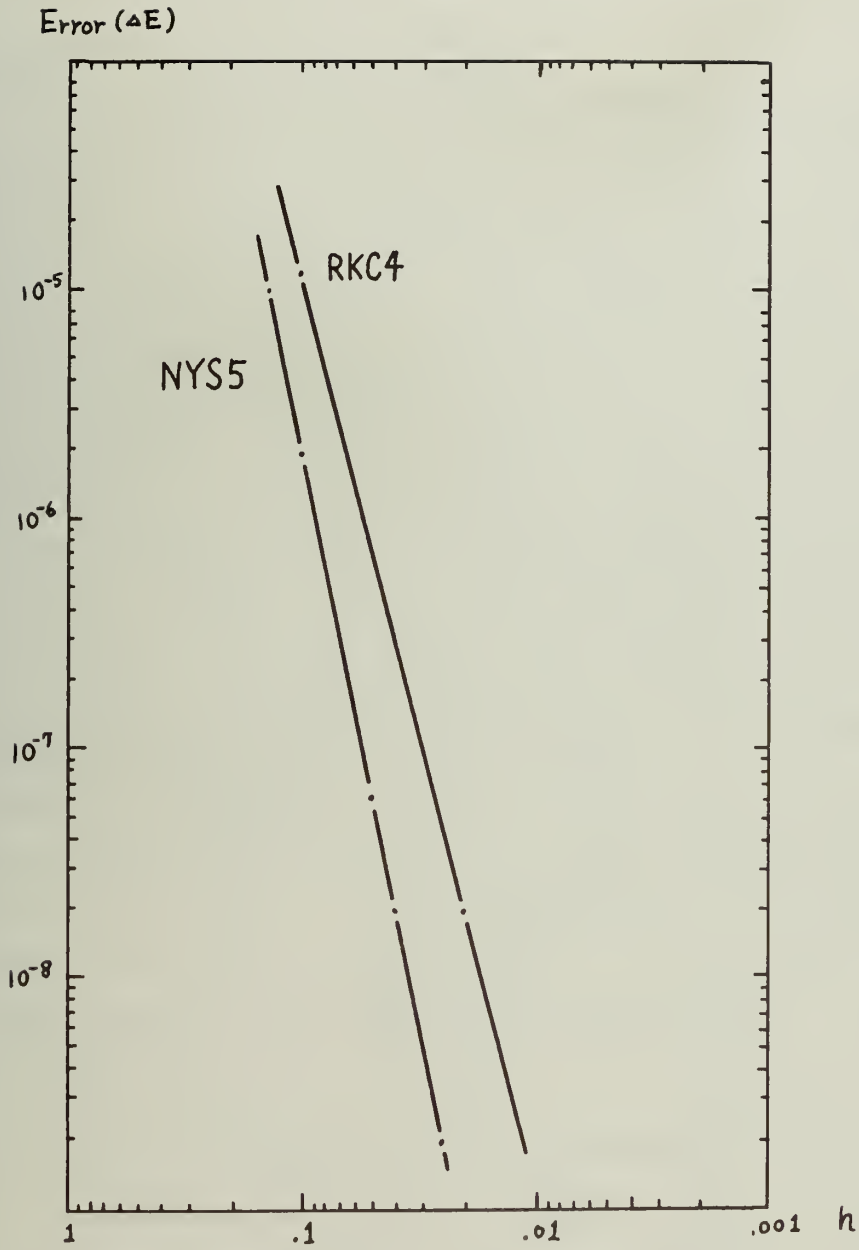


Fig. 4.1. Comparison of NYS5 and RKC4 (truncation errors).

This can be best understood by considering two zero temperature heat reservoirs; the end atoms lose their energy everytime they interact with the heat reservoirs and the lattice will be cooled off eventually. Some computational results are given in §6.1. We found that a more efficient energy transfer was possible by letting the end atoms move freely for several integration steps, that is, boundary crossing of the end atoms is examined at several integration steps. (Also refer to §5.3.) It is also possible to obtain a better contact by moving the heat reservoirs inward (applied pressure) so that more number of collisions takes place. JPW reported that this increased the number of collisions. We should note, however, that this inevitably changes the degree of nonlinearity of the lattice, since the average interatomic spacing is reduced. In our computation we did not apply any pressure to the lattice.

Nakazawa took a different approach by considering the Brownian motion of the end atoms directly. Namely he introduced the viscosity to the end atoms besides the random force and the nearest neighbor interaction. Hence the equation of motion is changed to:

$$\frac{d^2 y_1}{dt^2} = f(y_2 - y_1) - \mu_1 \frac{dy_1}{dt} + B_1(t) \quad (\text{left end})$$

$$\frac{d^2 y_n}{dt^2} = f(y_{n+1} - y_n) - f(y_n - y_{n-1}) \quad (n=2 \sim N-1)$$

$$\frac{d^2 y_N}{dt^2} = -f(y_N - y_{N-1}) - \mu_N \frac{dy_N}{dt} + B_N(t) \quad (\text{right end})$$

where

$$\overline{B_1(t)B_1(t')} = 2T_1 \delta(t-t')$$

and

$$\overline{B_N(t)B_N(t')} = 2T_N \delta(t-t') .$$

Nagazawa chose μ_1 and μ_N that yield the optimal contact between the lattice and the heat reservoirs for the highest mode of the lattice. (20)

4.4 Computer Facilities and Programs

The computer which we used for our numerical experiments is Burroughs B6700 system located at the Center for Advanced Computation at the University of Illinois. The word length is 48 bits with 39 bit mantissa. Its characteristics are implied by the following figures: addition time $.20\mu s$, multiplication time $2.00\mu s$ and division time $10.8\mu s$. (40) B6700 has a special architecture designed suitably for processing ALGOL language. It is not primarily designed for high speed scientific computations, but its flexible operating system (MCP) allows users to manipulate remote terminals, on-line monitoring, etc., without requiring much experiences in system programming on users' part. Fig. 4.2 shows the B6700 system as far as our computation is concerned.

Our programs are stored on a 9 track magnetic tape and are easily read on the disc memory. Editing of programs can be done from the remote terminals, from which an immediate access to the disc memory is possible. The remote terminal which we used is the Hazeltine 2000. It is a character display terminal (27 rows x 68 columns), having the cursor addressing feature. This latter feature allows users to write programs which plot curves (although very crude since its resolution is 25×60 points) while the main program is being executed. This is very convenient when we monitor what is going on in the program.

By making use of the terminal just described, we wrote our programs in a semi-interactive way. Some of the features of our programs are:

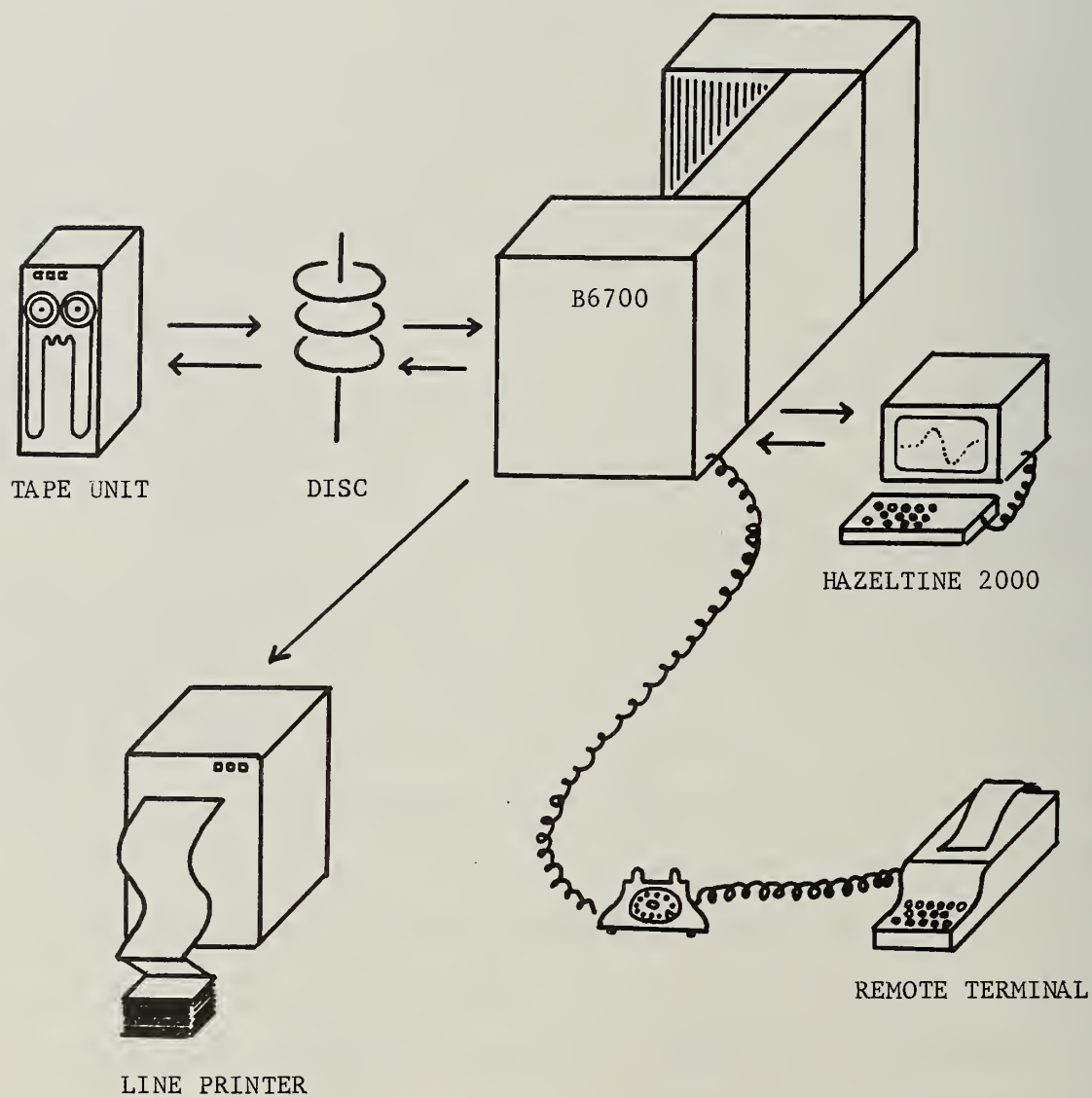


Fig. 4.2. Computer facilities.

- (1) A command to execute a program is given from a terminal. This terminal will be tied up to the program until the program is terminated.
- (2) Input parameters are fed from the terminal. There are also some options for printing only the desired variables such as the coordinates, velocities, temperature and flux.
- (3) Intermediate results are displayed on the terminal at an option. Time interval can also be set at which we require displays.
- (4) Programs can be terminated at any time by sending a command from the terminal if the user does not need it any more.
- (5) An interactive use of the terminal is possible only when the program reaches to the points at which it requires some information from the user. Therefore our programs are not interactive in the strict sense. But even semi-interactive programs of this level still enable us to use the computer system quite efficiently for the heuristic research.

Instead of creating a huge, complicated program that handles everything, we have made separate programs for considerably different tasks. Table 4.3 gives a list of programs which we have created.

4.5 Description of a Typical Program

As a typical example of our programs we describe SOL/XXIV that was written for computing the heat flux and the temperature distribution. A simple flow chart is given in Fig. 4.3. In this program the heat flux and the temperature are computed and printed (also on the terminal) at every 50 seconds. The temperature gradient is computed by the linear least-square interpolation. The entire program is in Appendix D.

Table 4.3
List of Programs

SOL/XXIV	heat conduction (JPW)
ZABUSKY	periodic boundary condition (Zabusky)
IMPACT	creation of solitary wave (JPW)
IMPACT2	creation of tail (JPW)
DISORDER	one impurity at $n=25$ (harmonic)
DISORDER2	impurities at $n=25\sim 50$ (harmonic)
DALT	impurities alternatively (harmonic)
BRKLIN	piecewise linear force
RESPONSE	cooling process of the lattice (JPW)
VISC	viscous ends (Jackson's problem)
RKC4	Runge Kutta Classical test
NYS5	Nyström test
SPHERE	hard sphere + harmonic
FPU	recurrence phenomena (cubic force)
FPU2	recurrence phenomena (quadratic force)
HAZELTINE	test program for the terminal
FPU3	recurrence phenomena (free ends)

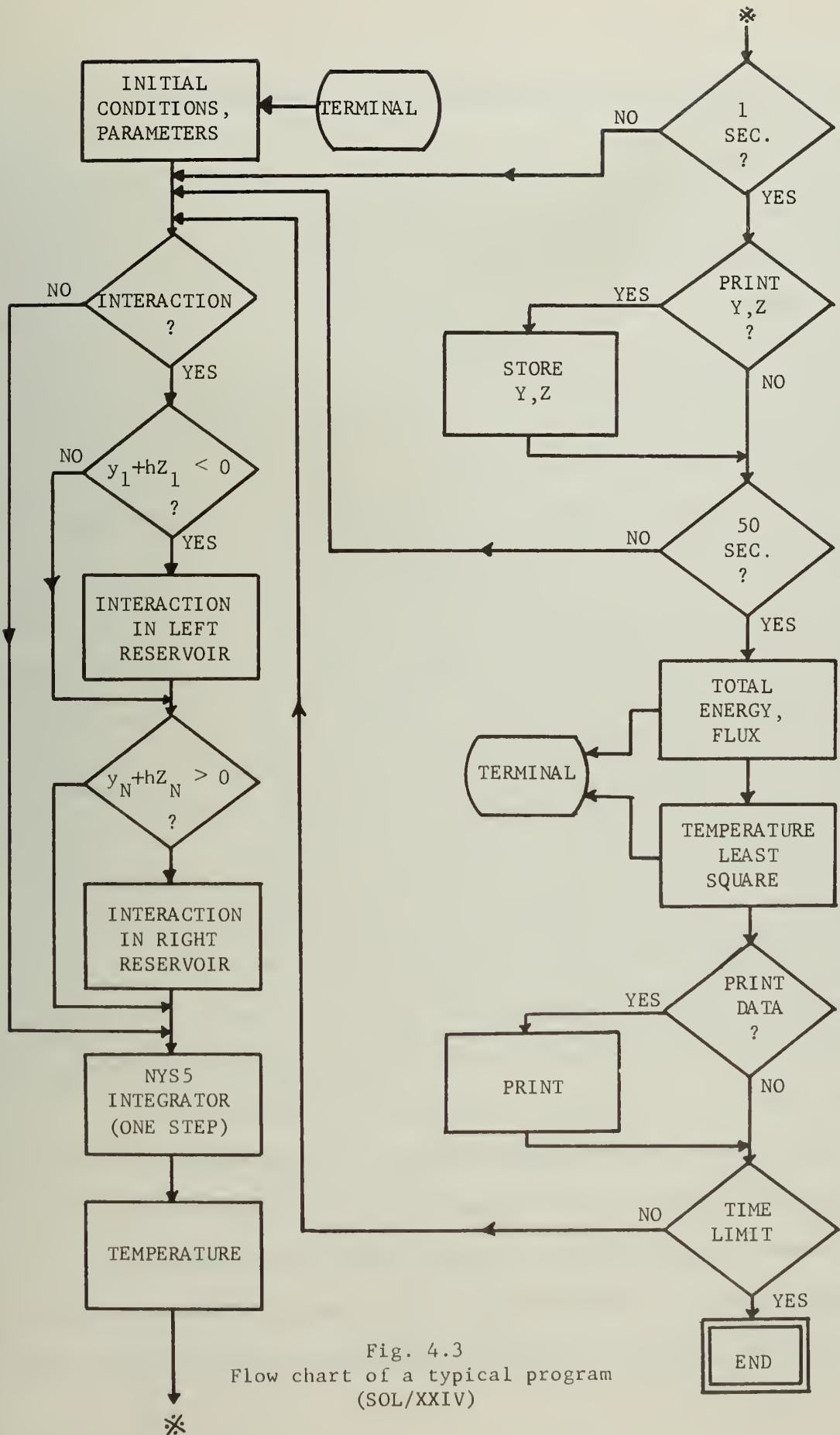


Fig. 4.3
Flow chart of a typical program
(SOL/XXIV)

CHAPTER 5. DYNAMIC PROPERTIES OF ANHARMONIC LATTICES

This chapter deals with the wave motions in the anharmonic lattices. Specifically JPW lattice (which is characterized by the force function $f(x) = x - 10x^2 + 66.7x^3$) is considered in full, but the piecewise-linear force model and the hard sphere plus linear force models are also treated. Since no analytical solutions are known, the numerical methods are employed and the results are compared with the analytical solutions in the continuum approximation whenever possible.

The solutions in Chapter 3 were considered in the special cases; the solitary waves and the periodic waves in the infinitely long lattices, or equivalently, under the periodic boundary condition. Most of the numerical experiments have been performed along this line.⁽³³⁾ In the heat conduction problem there are new factors. Firstly, the lattice is necessarily bounded by the heat reservoirs. Therefore the effect of the boundaries must be taken into account. Secondly, the initial condition is different from that for a pure solitary wave solution; we assume the impulse type interaction between the lattice and the heat reservoirs. In fact, an impulse produces an oscillatory wave packet together with a solitary wave. The main purpose of this chapter is to clarify the basic energy transport properties of the anharmonic lattices from the numerical experiments. Most of the results in this chapter have not been reported.

From §5.1 to §5.4 we consider solely the JPW lattice. In §5.1 we consider the creation of the solitary wave by the impulse. In §5.2 we will compare various boundary conditions and the reflection of the solitary waves therein. We will show that the fixed boundary is a perfect reflector but that the free boundary destroys the solitary waves. In §5.3

we will consider the two wave collision process. We discovered that the solitary wave slightly loses its energy in the collision process. We will also mention the wave propagation through the disturbances. In §5.4 we will discuss the behavior of the time averaged kinetic energy of the atoms when the waves propagate through the lattice. This quantity defines the local temperature in the thermal situation. In §5.5 and in §5.6 we will consider the piecewise linear force function and the hard sphere type force function, respectively. We will numerically show that the solitary wave can exist in these models.

The results obtained in this chapter will be used in Chapter 6 in understanding the heat conduction phenomena.

We should note that we will employ the coordinate space which is defined by the atom number n and the time t rather than the spatial coordinate x and the time t . The former definition corresponds to the Lagrangian coordinate system and the latter to the Eulerian coordinate system in hydrodynamics. The advantage of the former is that the atom number n is fixed all the time whereas the n^{th} atom itself moves in the one dimensional space. This difference is very important when we consider the collision process. The approach we took in deriving the partial differential equation in Chapter 3 relates the (n,t) space in the lattice with the (x,t) space in the continuum approximation.

5.1 Basic Dynamic Properties of JPW Lattice

5.1.1 Creation of the Solitary Wave by the Impulse

We discovered that an impulse applied to the end atom of the lattice produces a solitary wave and a tail. By the latter we mean a small wave packet which consists of high frequency waves. A typical profile of such

wave is given in Fig. 5.1a. Separation of the two parts was observed at an early time for the initial velocity greater than .08. If the initial velocity is small ($<.05$) separation was not observed within the limit of our lattice size ($N=100$). Such an example is also given in Fig. 5.1b. In this case the entire wave propagates as a (dispersive) wave packet. Presumably separation will take place after the wave propagates for a long distance. Zabusky also found a similar type of the wave as a solution of the KdV equation.⁽⁴¹⁾ Unfortunately, there is no analytical solution known for such composite (solitary wave plus tail) waves.

First we look at the solitary wave part. We performed numerical experiments with different initial velocities. Results are in Table 5.1. Fig. 5.2 shows the relation between the amplitude of the wave and the propagation velocity v . The solid curve is the theoretical prediction from the continuum approximation (3.29):

$$v^2 = C_0^2 \left(1 + \frac{\epsilon}{3}A + \frac{\mu}{6}A^2 \right)$$

with $C_0^2 = 1$, $\epsilon = 2 \times 10$, $\mu = 3 \times 66.7$ and $a = -A$. Experimental data are always located below the theoretical curve. This tendency becomes manifest as the amplitude increases. Apparently the truncated terms in the continuum approximation are responsible for this effect, since the wave form becomes sharper as the amplitude increases. Fig. 5.3 shows the relation between the initial velocity V_i and the propagation velocity v . We can derive an empirical formula $v = 1 + 1.85V_i$ in the range $[.1, .4]$.

5.1.2 Energy Concentration

Since the propagation velocity of the solitary wave is much faster than that of the tail, we can calculate the energy contained in each part separately. The energy of the n^{th} atom is defined as

Table 5.1. Dynamic Properties of Solitary Waves

V_i	Amp.	V	E_{sol}	E_{tail}	$E_{sol}(\%)$	h	Error
.08	.0364	1.13	.00292	.00028	91.1	.02	.5 10^{-8}
.1	.0465	1.19	.00467	.00033	93.4	.05	.9 10^{-5}
.2	.0900	1.39	.01960	.00040	98.0	.025	<.5 10^{-8}
.3	.1252	1.57	.04455	.00045	99.0	.05	.2 10^{-6}
.4	.1550	1.75	.07952	.00048	99.4	.05	.6 10^{-6}
.5	.1819	1.89	.12450	.00050	99.6	.025	.8 10^{-7}
.6	.2066	2.02	.17940	.00060	99.67	.05	.3 10^{-5}
.8	.2482	2.27	.31931	.00069	99.8	.05	.15 10^{-4}
1.0	.2840	2.51	.49920	.00080	99.99	.025	.6 10^{-5}
1.2	.3199	2.67	————	————	————	.1	————
1.5	.3640	2.97	————	————	————	.1	————

V_i : initial velocity

Amp: amplitude of the wave

V: propagation velocity of the wave

E_{sol} : total energy in the solitary wave

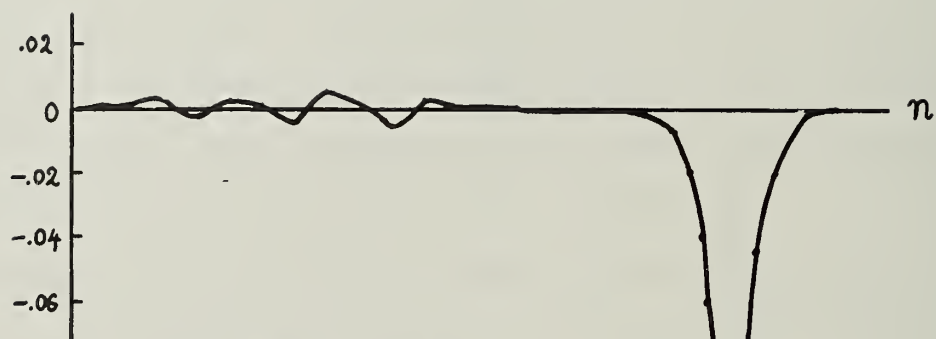
E_{tail} : total energy in the tail

$E_{sol}(\%)$: $E_{sol} / (.5 V_i^2)$

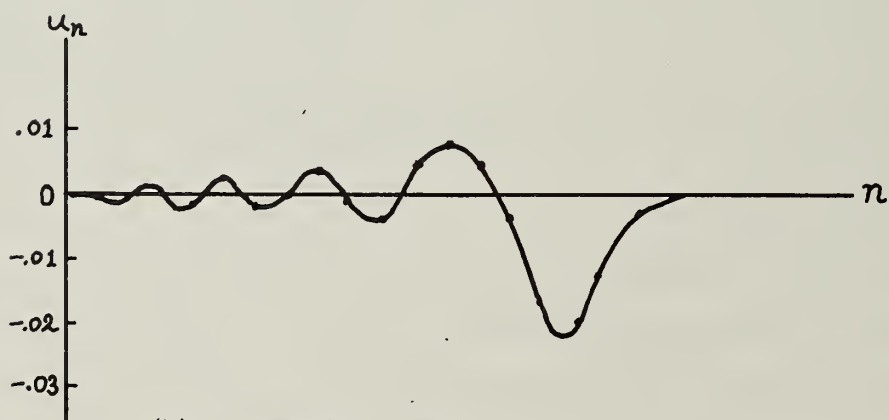
h: integration step

Error: numerical error in total energy

———— means that such quantity was not computed.



(a) $V_i = .2, t = 15$



(b) $V_i = .05, t = 15$

Fig. 5.1. Typical profiles of waves created by impulse.

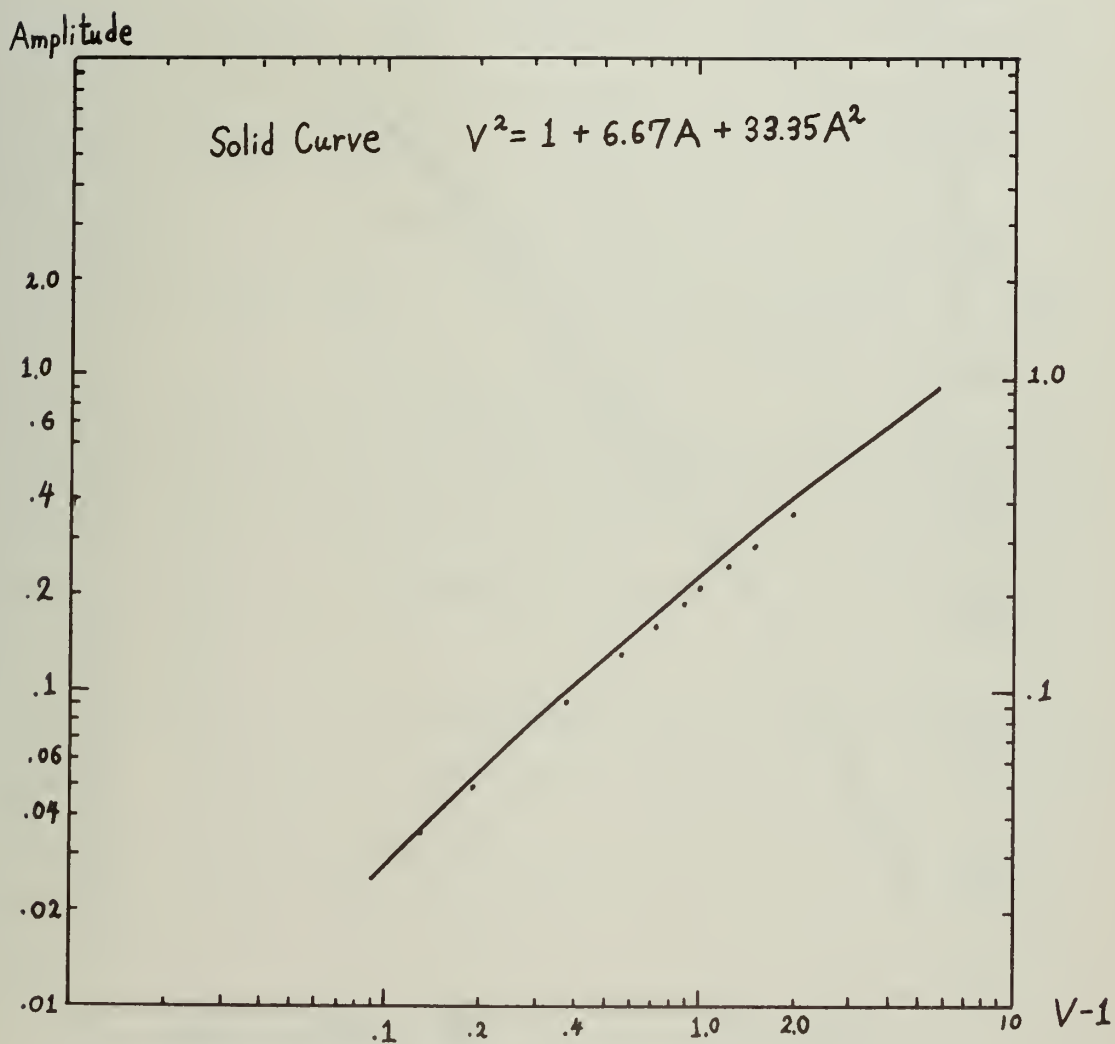


Fig. 5.2. Velocity vs amplitude relation.

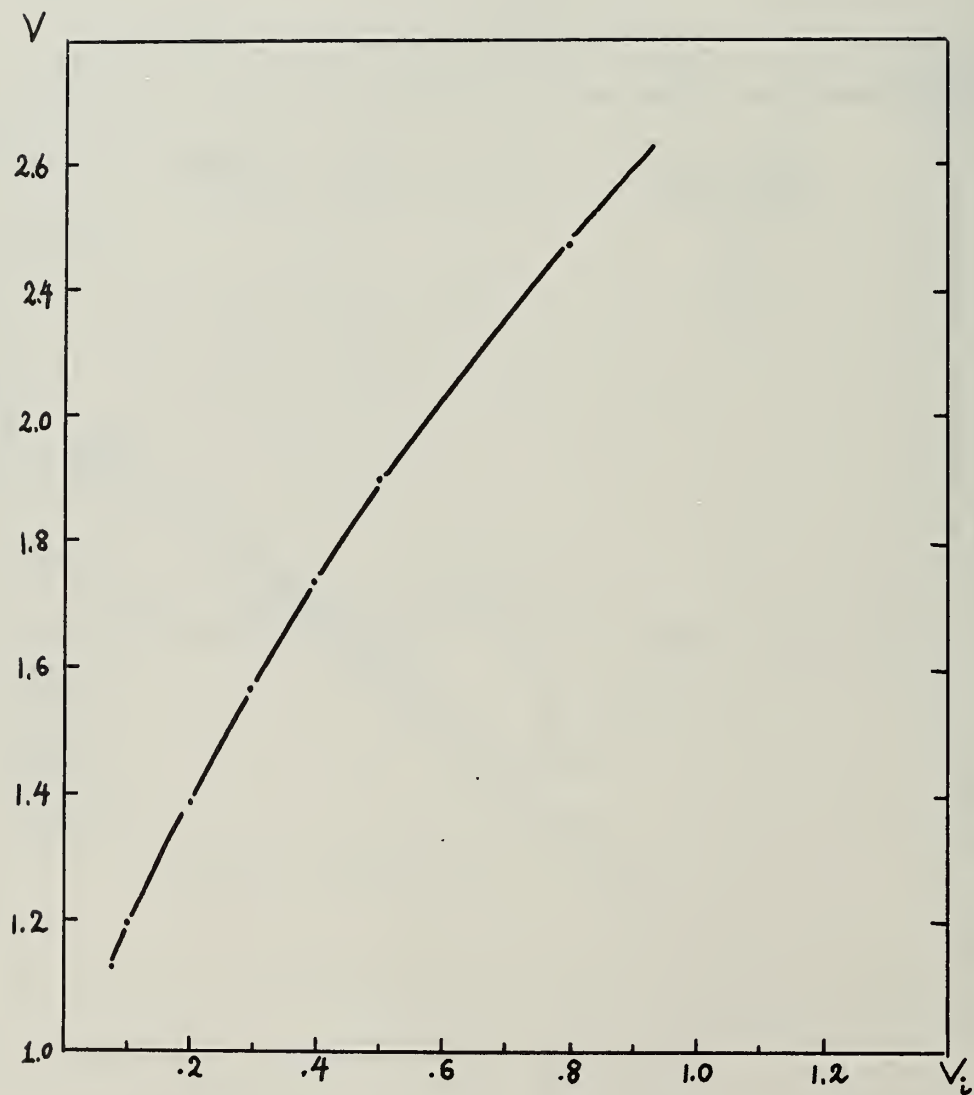


Fig. 5.3. Initial velocity vs propagation velocity.

$$E_n = \frac{1}{2} \dot{y}_n^2 + \frac{1}{2} [V(y_{n+1} - y_n) + V(y_n - y_{n-1})] \quad (5.1)$$

where $V(y_{n+1} - y_n)$ is the potential energy stored in the spring connecting the n^{th} and $n+1$ st atoms. Results are in Fig. 5.4. Numerical data for the JPW lattice are also given in the fourth column of Table 5.1. The stronger the nonlinearity is, or the larger the amplitude is, the more fraction of the energy is concentrated in the solitary wave, although the energy in the tail itself also increases. Fig. 5.5 is a typical example of the energy distribution in the JPW lattice. Fig. 5.6 shows the relation between the energy and the propagation velocity. From this graph we can obtain an empirical formula which is similar to $E = mv^2/2$:

$$E_s = M_s (v-1)^2/2 \quad (5.2)$$

where $M_s = .24 (L+.35(v-1)^2)$ (effective mass!).

It is obvious from the above results that the anharmonic lattice can transmit energy more efficiently than the harmonic lattice because of the nondispersiveness and the high propagation velocity of the waves therein.

5.1.3 Tail Part

As we mentioned in 5.1.1 an oscillatory wave is always created with a solitary wave. Its amplitude is very small compared with that of the solitary wave which it accompanies with. We can assume that the tail is the harmonic dispersive wave. This was verified by the following numerical experiment:

- (1) Create a solitary wave and a tail with an impulse and let them propagate until they are separated from each other;
- (2) erase the solitary wave;
- (3) reverse the direction of the time and perform the numerical integration backward until $t=0$;

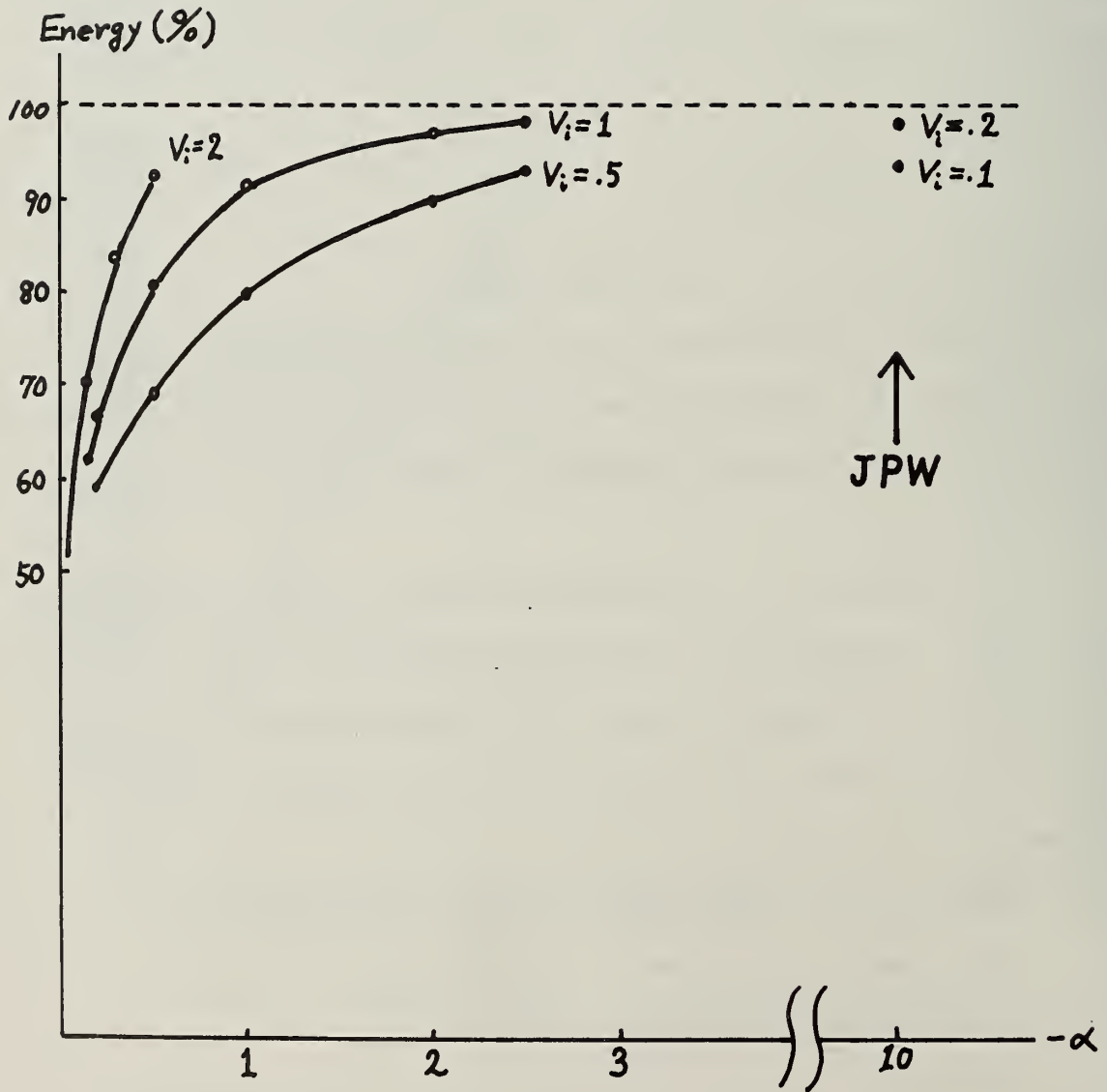


Fig. 5.4. Energy concentration in solitary wave (%).

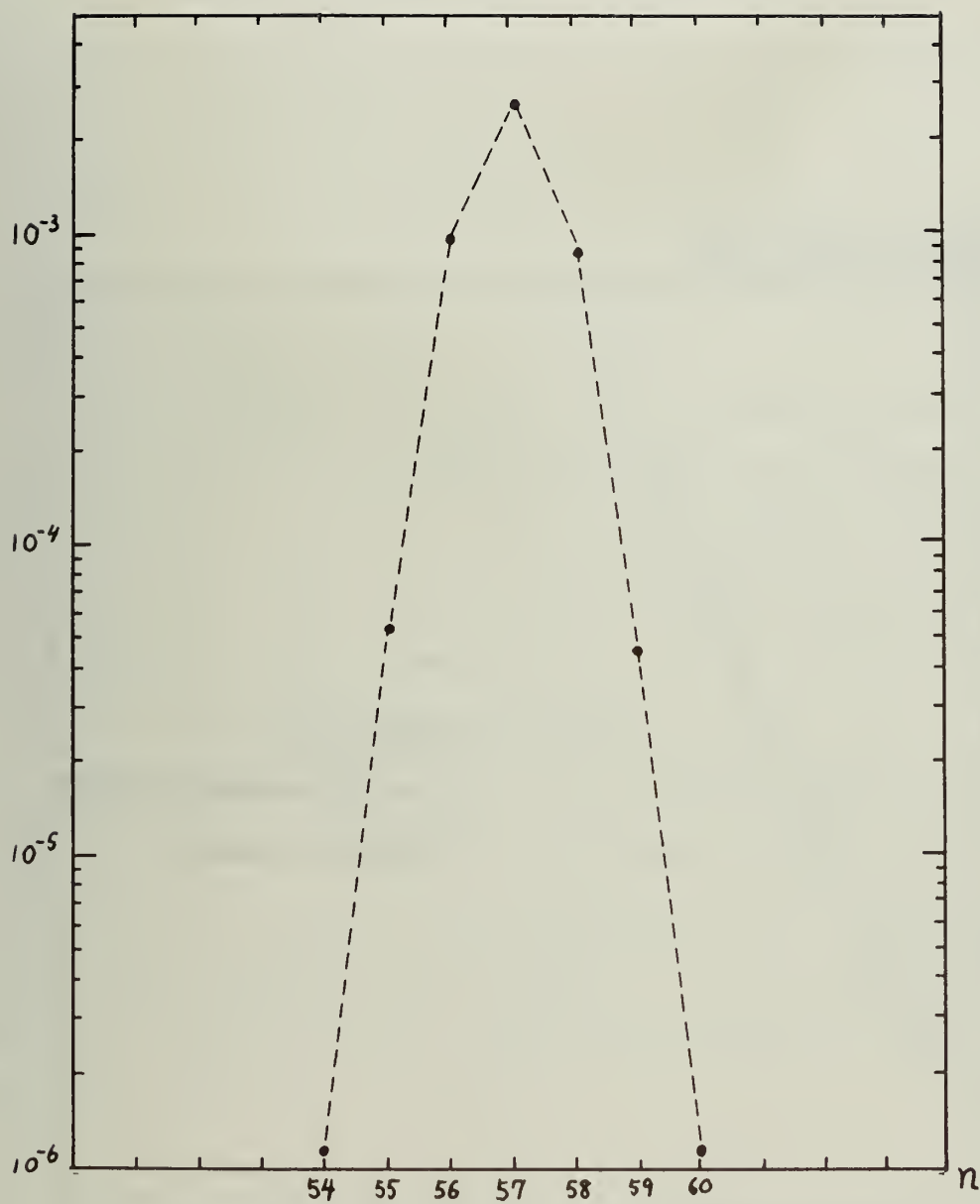


Fig. 5.5. Typical energy distribution in solitary wave.
 $V_i = .2$, $t = 37$, $h = .05$, $\Delta E = .5 \times 10^{-7}$.

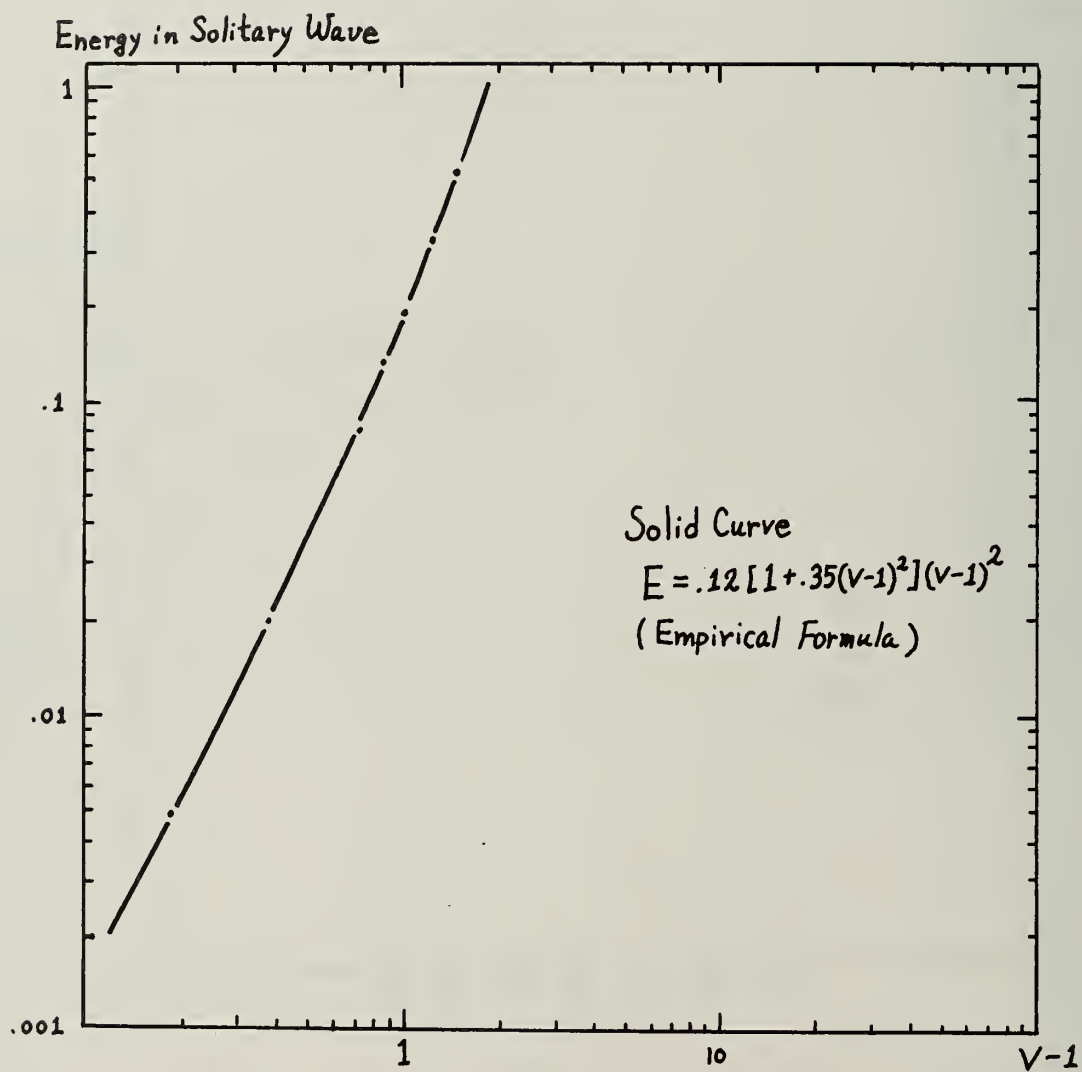


Fig. 5.6. Energy vs propagation velocity relation for solitary waves.

- (4) change the force function to the linear form and reverse the time again. The tail will propagate toward right;
- (5) compare the wave form of the harmonic tail with the form of the anharmonic tail at the corresponding time.

Fig. 5.7 shows the result; there is no appreciable difference between them. The phase delay is due to the different initial condition and not due to the different propagation velocities.

The tail propagates very slowly since it consists of high frequency components. It is quite suggestive that the interaction between the lattice and the heat reservoir always produces two waves of completely different characters; we depend on this fact when we consider the origin of the temperature gradient (Chapter 6).

5.1.4 Mode Spectrum of Solitary Waves

Since the solitary wave is formed due to the coupling of the modes, it is interesting to see how the mode spectrum changes as the wave propagates. An impulse applied to the end of the lattice gives the initial energy distribution as is shown in Fig. 2.2. The time evolution of the spectrum is shown in Fig. 5.8. The lattice consists of 25 atoms with free boundaries. The initial velocity is .5.

5.2 Boundary Effects

We examined several types of boundary conditions. The solitary waves were injected from the left for all experiments.

5.2.1 Fixed Boundary (Fig. 5.9)

Solitary waves are reflected completely. There is no appreciable energy left at the boundary, but the phase of the wave is somewhat advanced. (See §5.3.)

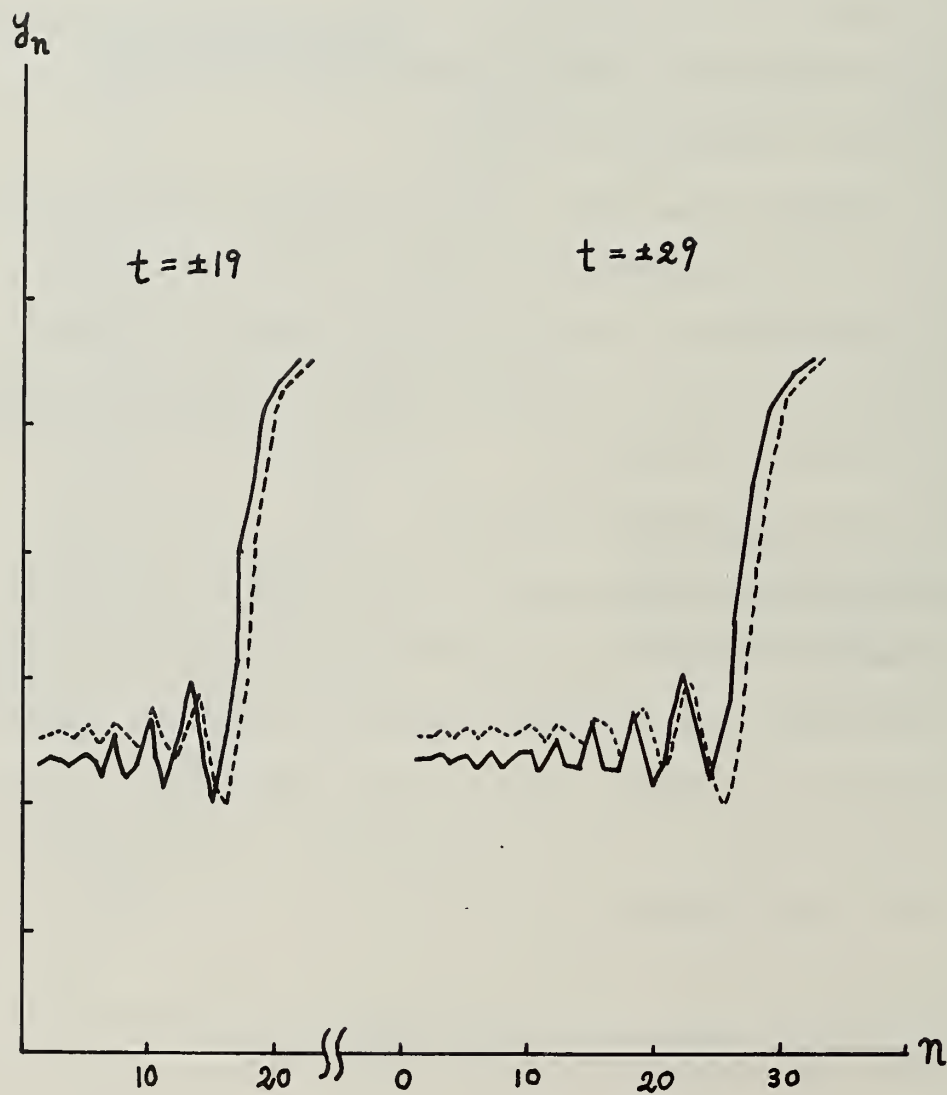


Fig. 5.7. Comparison of harmonic tail (-----) and anharmonic tail (—————).

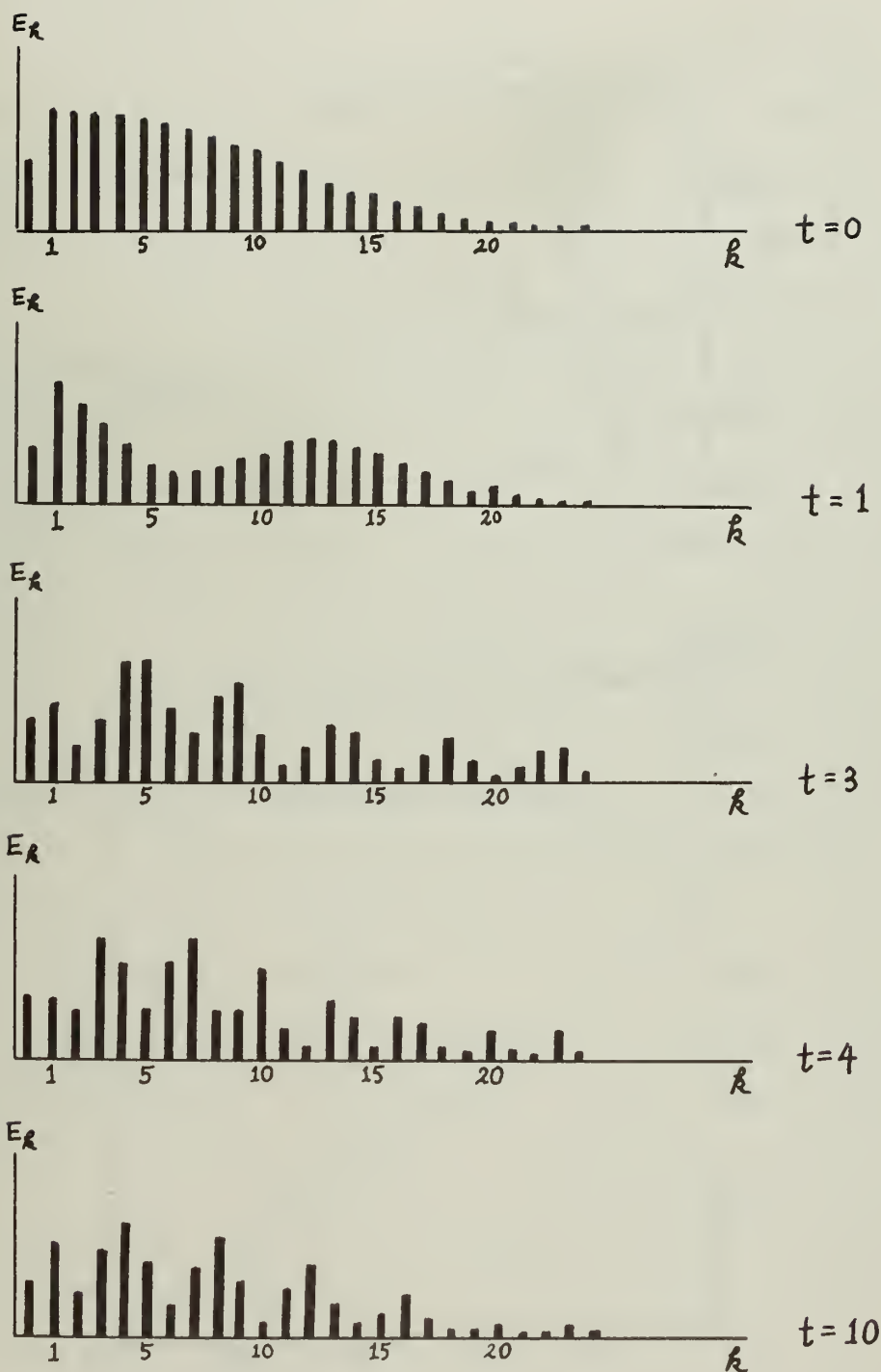


Fig. 5.8. Mode spectra ($N=25$) of solitary waves.

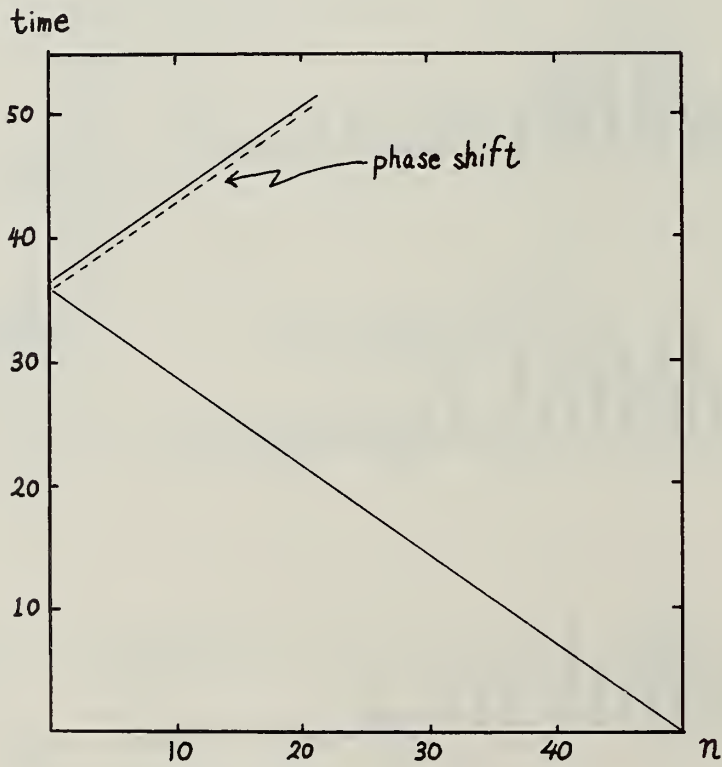
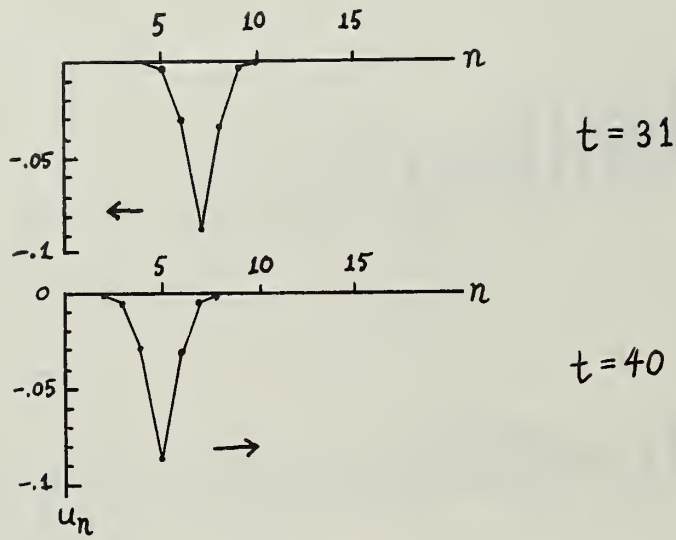


Fig. 5.9. Reflection of solitary wave at fixed boundary.

5.2.2 Free Boundary (Fig. 5.10)

The solitary waves decay at the free end when the amplitudes are small, whereas those with large amplitudes can be reflected. This difference may be explained in the following way. When the solitary wave reaches the end of the lattice, atoms near the end tend to travel in the same direction, resulting in the expansion of the lattice there. This newly created expansion wave can propagate through the lattice back again as a solitary wave only when the force (in the positive region of the displacement) becomes stiff as the amplitude increases. In the case of the JPW lattice, however, the force at first becomes limp due to the negative quadratic nonlinearity, then it becomes stiff again due to the cubic nonlinearity which dominates the quadratic one. Hence there is a threshold of the amplitude below which the solitary waves become unstable. To make this point clear we also performed a numerical experiment with the negative impulses applied to the JPW lattice. Fig. 5.11 shows the responses of the lattice to various inputs. The critical velocity turned out to be $V_i = .3$.

5.2.3 Heat Reservoir Type Boundary

In this boundary condition, the coordinate of the end atom is checked at every m integration steps. If the end atom is found to be inside the heat reservoir a new velocity is assigned. We performed the numerical experiments with various m . Since we are concerned with the boundary effect in this chapter rather than the thermal properties, we chose the predetermined values for V_i and V_r , where V_r is the velocity with which the end atom is returned. Specifically, $V_i=1$ and $V_r=.1$. Results are in Fig. 5.12 a-e. The amplitude of the reflected wave decreases as m increases. If $m=1$ the end atom is effectively frozen at the boundary, therefore the boundary condition is very similar to the fixed boundary condition. As m increases,

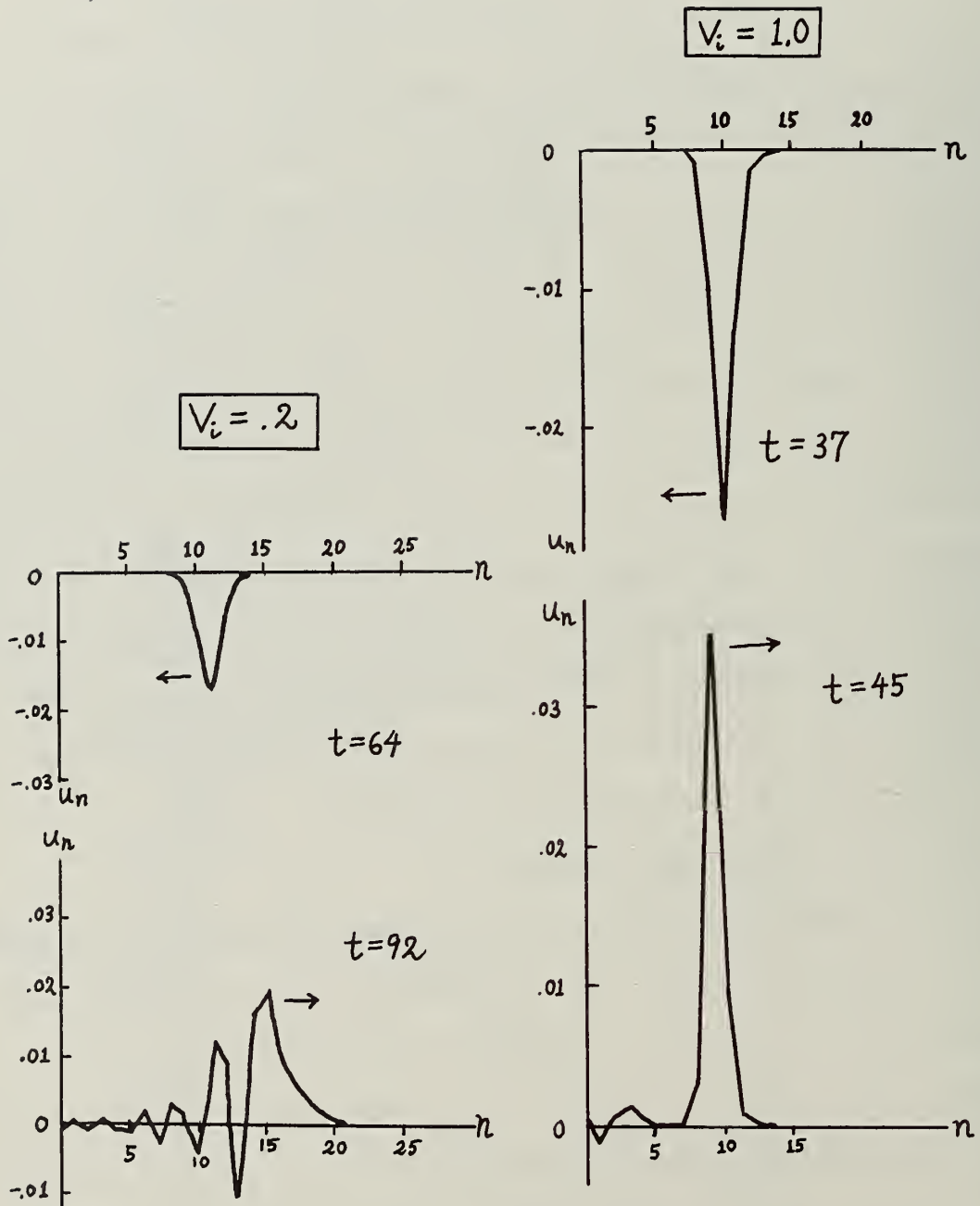


Fig. 5.10. Reflection of solitary waves at free boundary.

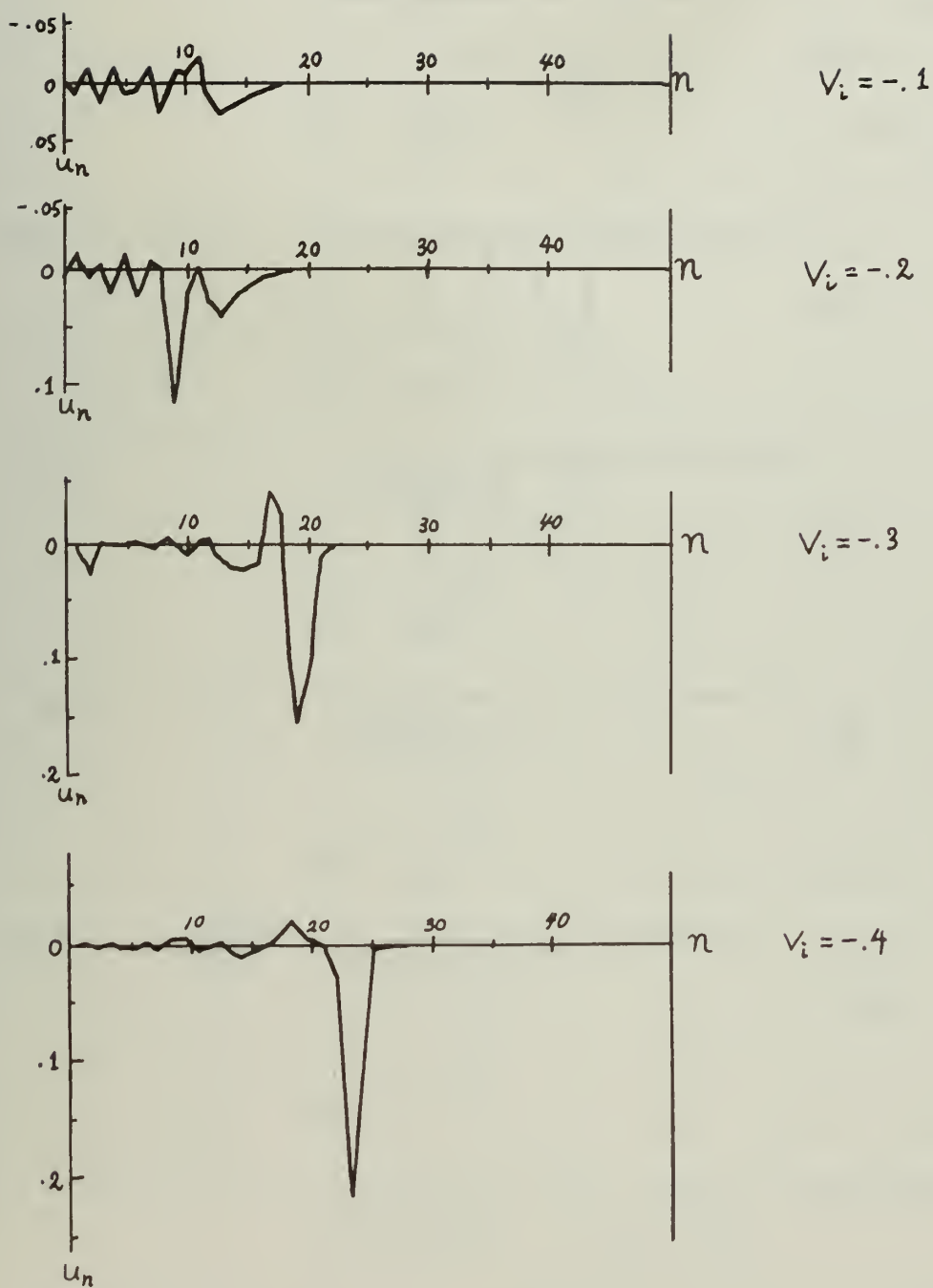


Fig. 5.11. Responses to negative initial impulses ($t=20$).

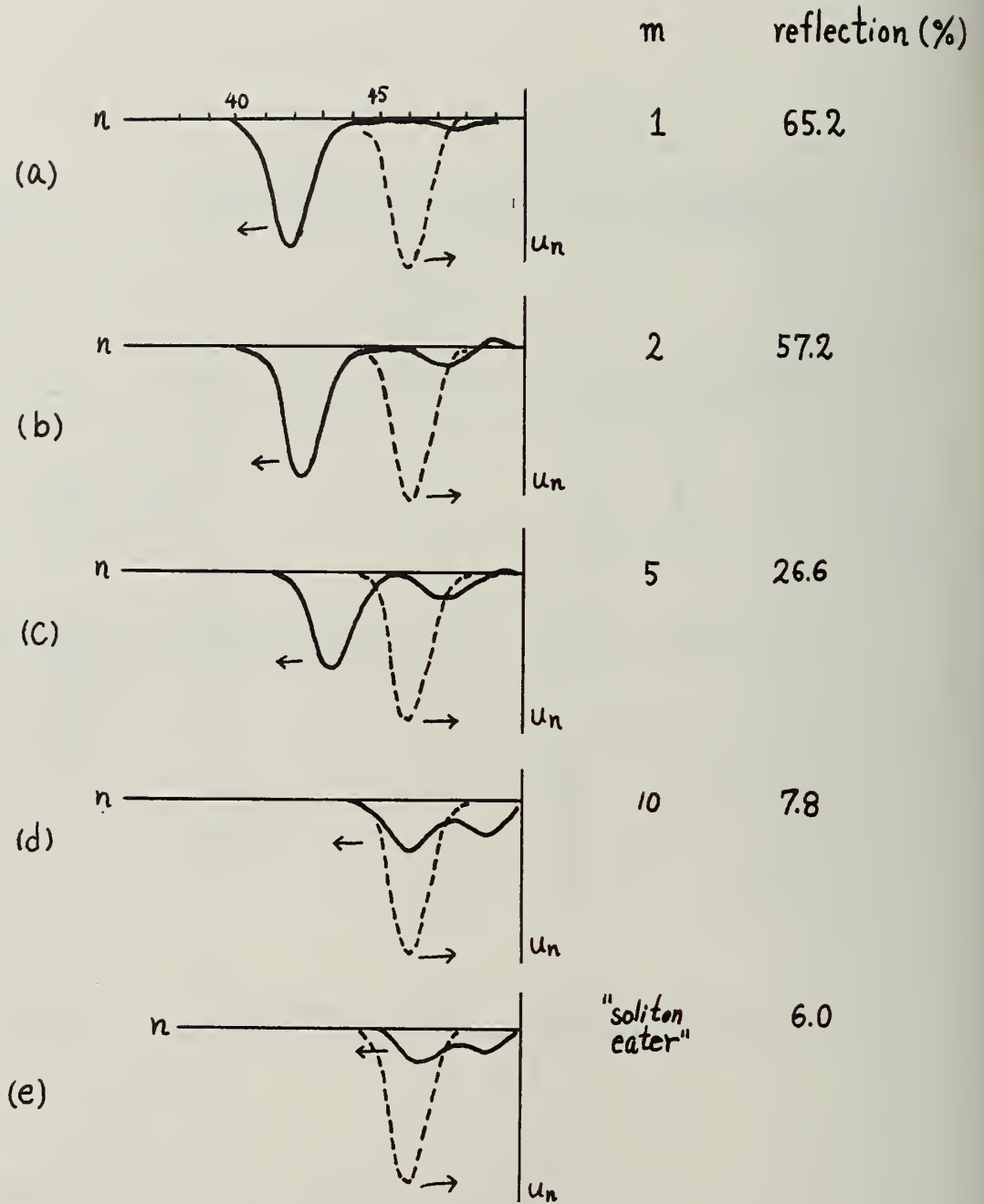


Fig. 5.12. Heat reservoir type boundary
 Broken curves: incoming wave
 Solid curves: reflected wave
 $V_i = 1$, $V_R = .1$.

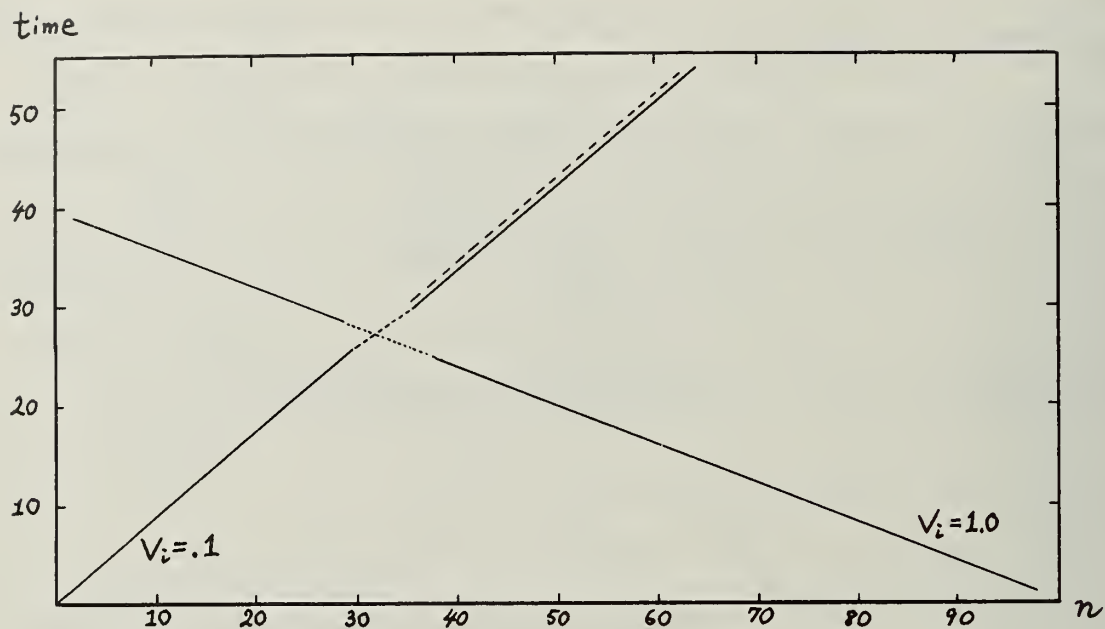
the end atom can receive more energy from its left neighbor before it interacts with the heat reservoir, hence more energy is exchanged. We also examined the boundary condition (called "soliton eater") which supposedly yield the most efficient energy exchange for the solitary waves; the end atom does not interact with the reservoir until its velocity reaches the maximum value. The result is shown in Fig. 5.12e. The effect of the boundary condition on the heat flux will be discussed in Chapter 6.

5.3 Collision Process of Solitary Waves

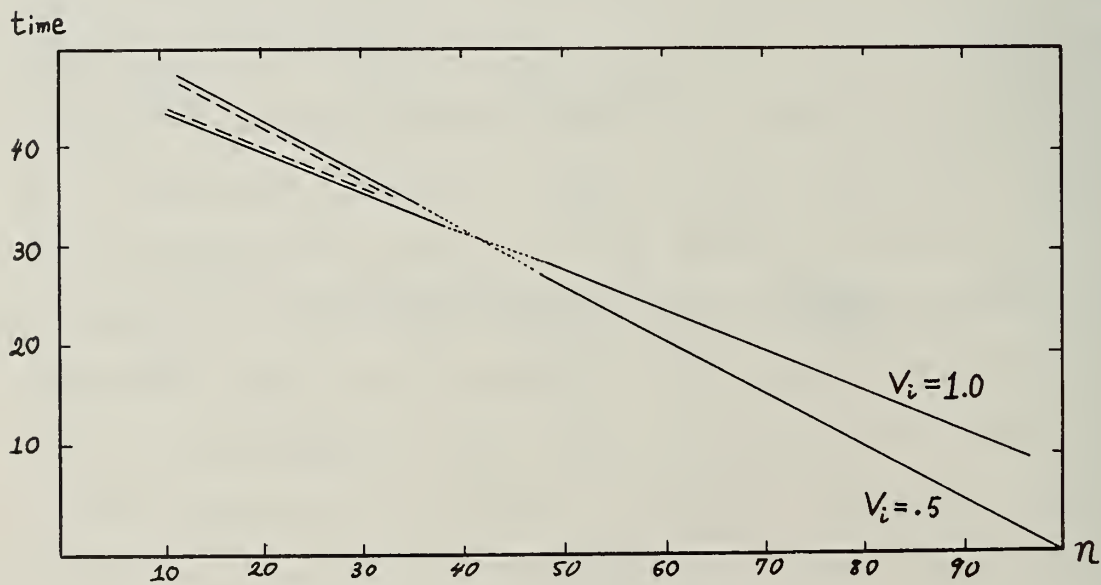
5.3.1 Phase Shift in Two Wave Collision Process

It was theoretically shown that the phase shift occurs in the two wave collision process in Toda's lattice (§3.5). In the JPW lattice the phase shift was observed experimentally; both waves were advanced after a head-on collision, whereas the faster wave was advanced and the slower wave was retarded after a take-over collision (Fig. 5.13). The amount of the phase shift was larger for the small amplitude wave in both types of collision. This seems to indicate that the motion of "the center of the mass" is not affected by either type of collision, the theoretical result obtained by Wadati and Toda for the KdV equation.⁽⁴²⁾ We should note that the above mentioned phase shift is considered in (n,t) space. Since the lattice itself is contracted toward the center, the phase shift is less obvious in (x,t) space. The phase retardation for the harmonic lattice, reported by JPW, is due to this difference⁽²¹⁾; there is no phase shift in (n,t) space.

The phase shift observed when the solitary wave hits the fixed boundary (5.2.1) can be explained in terms of the two wave collision process. If two solitary waves of equal amplitude travel in the opposite direction in such



(a) Head-on collision.



(b) Take-over collision

Fig. 5.13. Collision process of two solitary waves.

a way that a collision takes place exactly at the location of, say, m^{th} atom, the m^{th} atom never moves. Hence the fixed boundary condition is strictly satisfied (Fig. 5.14a). We can further conclude from the numerical results in 5.2.1 that the solitary waves lose no appreciable energy in a collision process which is equivalent to the fixed boundary condition.

5.3.2 Energy Loss

We can extend the above discussion to consider a different initial phase relation of two waves. Suppose that a collision takes place in the middle of two atoms. Such type of collision is equivalent to the reflection of the solitary wave at the fixed boundary, except that the interaction force at the boundary is twice as strong as that at all other places (Fig. 5.14b). Since the lattice becomes inhomogeneous, we can expect that the solitary wave may be deformed. We performed a numerical experiment on the two wave collision process along this line, and discovered that some of the energy is actually left at the site of a collision (Fig. 5.15). There are 50 atoms in the lattice, two end atoms having the initial velocities, .5 and -.5. A collision takes place between $n=25$ and $n=26$. The amount of the energy taken from the solitary waves is very small (.3% of the initial energy), but this is far above the numerical error. This numerical experiment was performed twice with different integration steps (i.e. .02 and .01); both gave the same results within the numerical errors. Hence the energy loss is not due to the numerical integration scheme. This newly created wave consists of high frequency components and is assumed to spread out in the entire lattice at $t = \infty$. Obviously the continuum approximation cannot treat such waves properly.

This fact may seem contradictory to the theoretical results because in Toda's lattice the only effect of a collision is a phase shift.⁽³²⁾ In

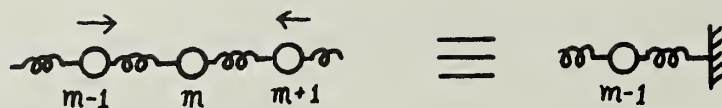


Fig. 5.14a. Fixed boundary

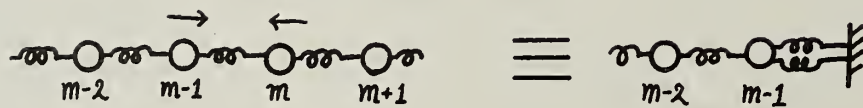
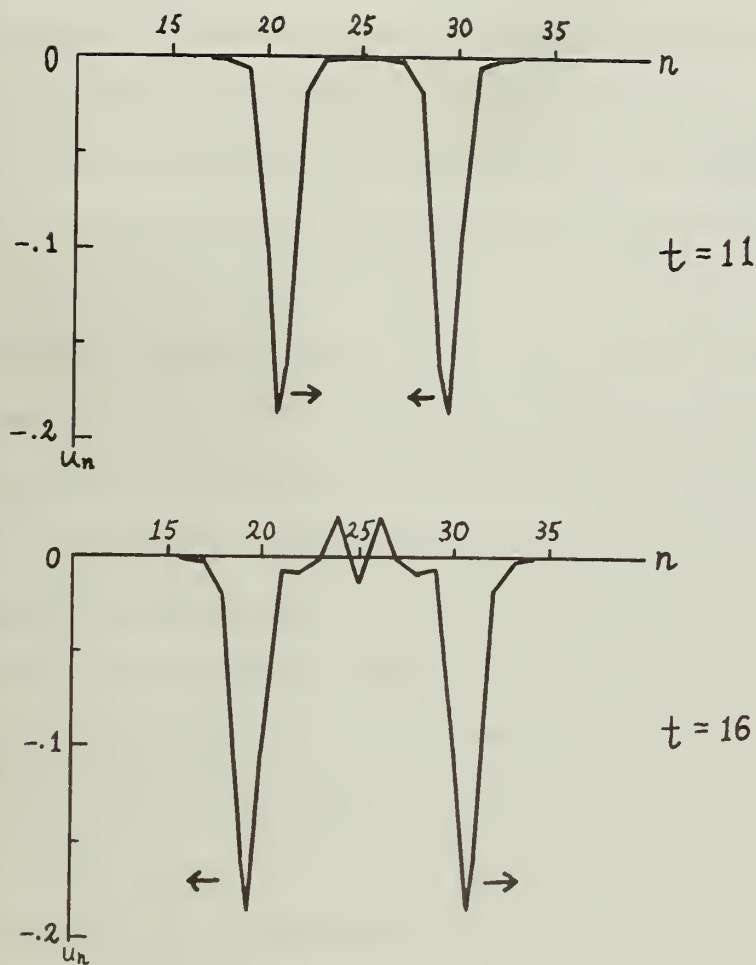


Fig. 5.14b. Another type of collision process.



$t=16$				
n	U_n		E_n	
	$h = .02$	$h = .01$	$h = .02$	$h = .01$
18	-.01736568	-.01736566	.00009400	.00009400
19	-.15784123	-.15784116	.02532067	.02532063
20	-.10197037	-.10197044	.09260386	.09260386
21	-.00731625	-.00731626	.00607652	.00607653
22	-.00756556	-.00756556	.00004459	.00004459
23	-.00259986	-.00259987	.00005328	.00005328
24	-.01865858	-.01865858	.00011343	.00011343
25	-.01257805	-.01257805	.00015234	.00015234
ΔE			.000000056	.000000002

Fig. 5.15. Energy loss in a collision process.

fact, the theory states that two solitary waves are shown to exist asymptotically ($t=\pm\infty$). But there are some other terms in the expanded form of Toda's solution, which vanish asymptotically. These terms are neglected in the theoretical argument. Note that these terms arise in the process of approximating the solution, not the equation. In our numerical experiments, two solitary waves are created at both ends of the lattice, between which there is no disturbance initially. Therefore the initial conditions are different in these two cases. As we mentioned before the wave created in a collision process will disappear as $t \rightarrow \infty$, if we assume the lattice of infinite length; asymptotically there are only two solitary waves.

The solitary waves in all collision experiments propagated after the collision without any decay. No decrease of the propagation velocity due to the energy loss was noticeable. We will show in §5.6 that the energy loss in a collision is more obvious for the hard sphere type force function.

In the thermal situation collisions can take place at any location of the lattice with equal probability. Also the energy loss, although exists, is negligible in the small sized lattice. Therefore we can summarize that the only important effect of the collision in our model lattice (JPW lattice) is that the propagation velocity of the solitary waves is effectively increased due to the phase shift.

5.3.3 Effect of the Disturbances

There is a question as to the propagation of the solitary wave when the disturbances (that is, the incoherent motion of the lattice) exist. Since the solitary wave is in the sea of disturbances under such circumstances, it is very difficult to isolate the energy in the solitary wave part and to measure its change. The only possible way is to observe the propagation velocity. As we discussed in §5.1, the solitary wave is

uniquely characterized by its velocity. Therefore any decrease of the velocity means that the energy is being lost. Fig. 5.16 shows an example. this figure was obtained by JPW, but it was not publicized in their report^{*}. (21) As we can see in Fig. 5.16, the velocity change is mainly due to collisions; the original velocity is regained after each collision. Hence we conclude that the interaction between the solitary waves and the disturbances is negligible for the lattices of order 100 atoms or so.

This does not mean, however, that no such interaction is possible. For example, if the lattice size is quite large the solitary wave may lose significant amount of its energy due to the interaction with the disturbances^{**} as well as due to many collisions with other solitary waves. As for the solitary waves of very small amplitude, we do not have any way to distinguish them from the disturbances.

5.4 Time Averaged Kinetic Energy

We define this quantity as follows:

$$K_n(t) = \frac{1}{t} \sum_{k=1}^M \dot{y}_n^2(k\Delta t) \quad (5.3)$$

where M is the number of time steps and $t = M\Delta t$. This quantity gives the local temperature when the lattice interacts with the heat reservoirs and $M \rightarrow \infty$. We calculated $K_n(t)$ for the impulse type initial condition. We considered both the harmonic and the anharmonic lattices.

^{*}The author is indebted to E. A. Jackson for this figure.

^{**}Saito et al. reported that a significant decrease of the velocity was observed for the solitary wave in Toda's lattice.⁽⁴³⁾

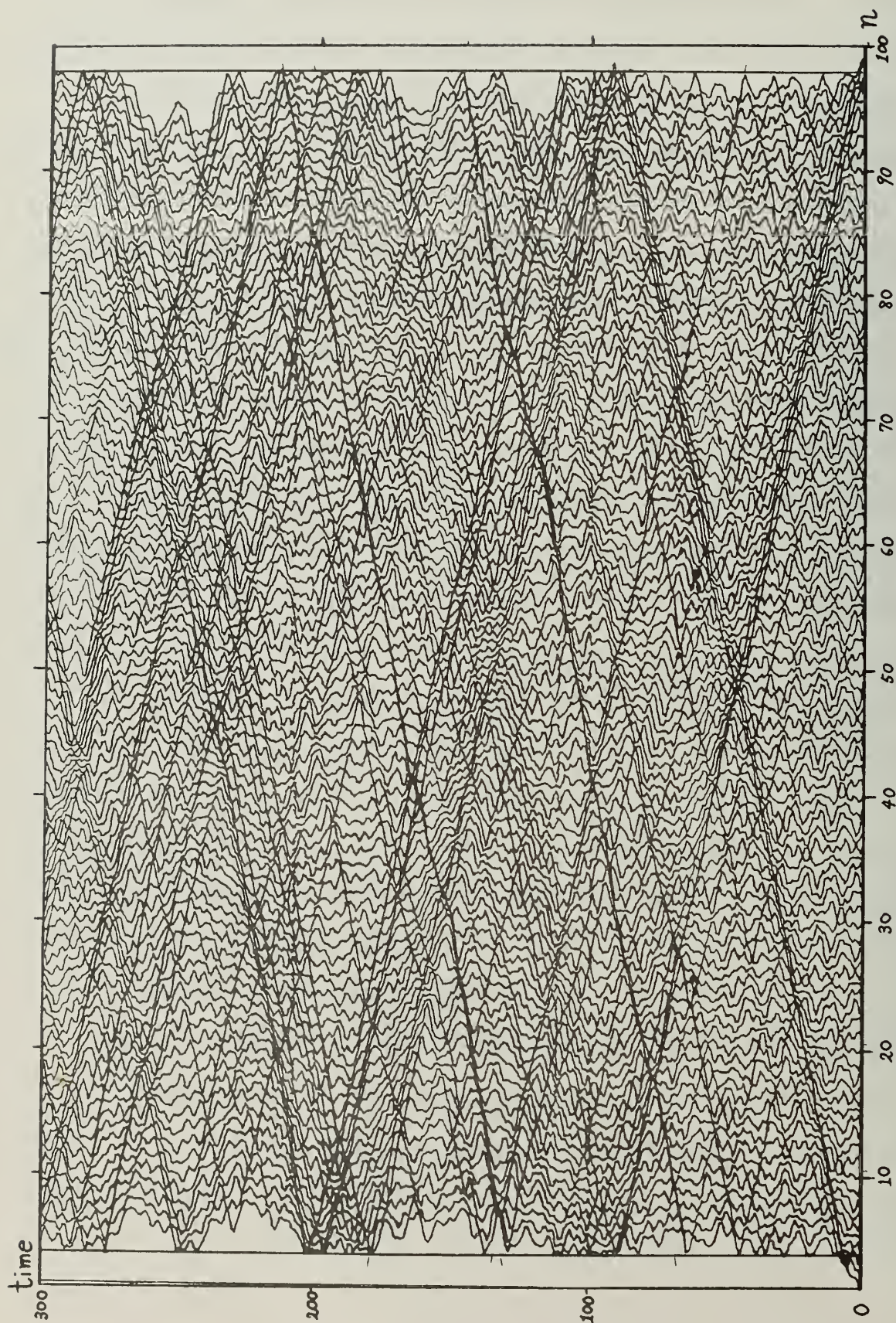


Fig. 5.16. Displacement of atoms in JPW lattice
($N=100$, $t=0 \sim 300$).

5.4.1 Harmonic Lattice (Dispersive Wave Packet)

As we discussed in Chapter 2 the created wave packet is very dispersive. That is, each component of the normal modes propagates at its own group velocity. Consequently $K_n(t)$ is a decreasing function of n for a fixed time t (Fig. 5.17a).

5.4.2 Anharmonic Lattice (Solitary Wave Plus Tail)

The solitary wave gives a uniform distribution as far as it has propagated. The tail, on the other hand, gives a decreasing contribution to $K_n(t)$ due to its dispersiveness. The resulting distribution is shown in Fig. 5.17b ($V_i=.1$) and in Fig. 5.17c ($V_i=.05$). The latter is a non-separating wave packet case. A sharp drop of $K_n(t)$ in Fig. 5.17b shows the location of the solitary wave.

5.4.3 Temperature Holes

We discovered that $K_n(t)$ for a two wave collision process has a dip around the site of the collision (Fig. 5.18a,b). This is partly due to the concentration of the spring; the kinetic energy is transferred to the potential energy when two waves collide. Obviously this effect is independent of the type of the force function, and in fact the same thing happens in the harmonic lattice (Fig. 5.18c,d). For the purpose of removing this spurious dip from $K_n(t)$ we experimentally defined the temperature in terms of the total energy. Although the temperature hole disappears in the harmonic lattice with the new definition of the temperature, it still remains in the anharmonic lattice (Fig. 5.18e,f). Hence we must conclude that the phase shift of the solitary waves is also responsible for the temperature hole; both waves are effectively accelerated during the collision process, contributing less to the local temperature. In the thermal situation the temperature holes can occur at any location of the lattice with an

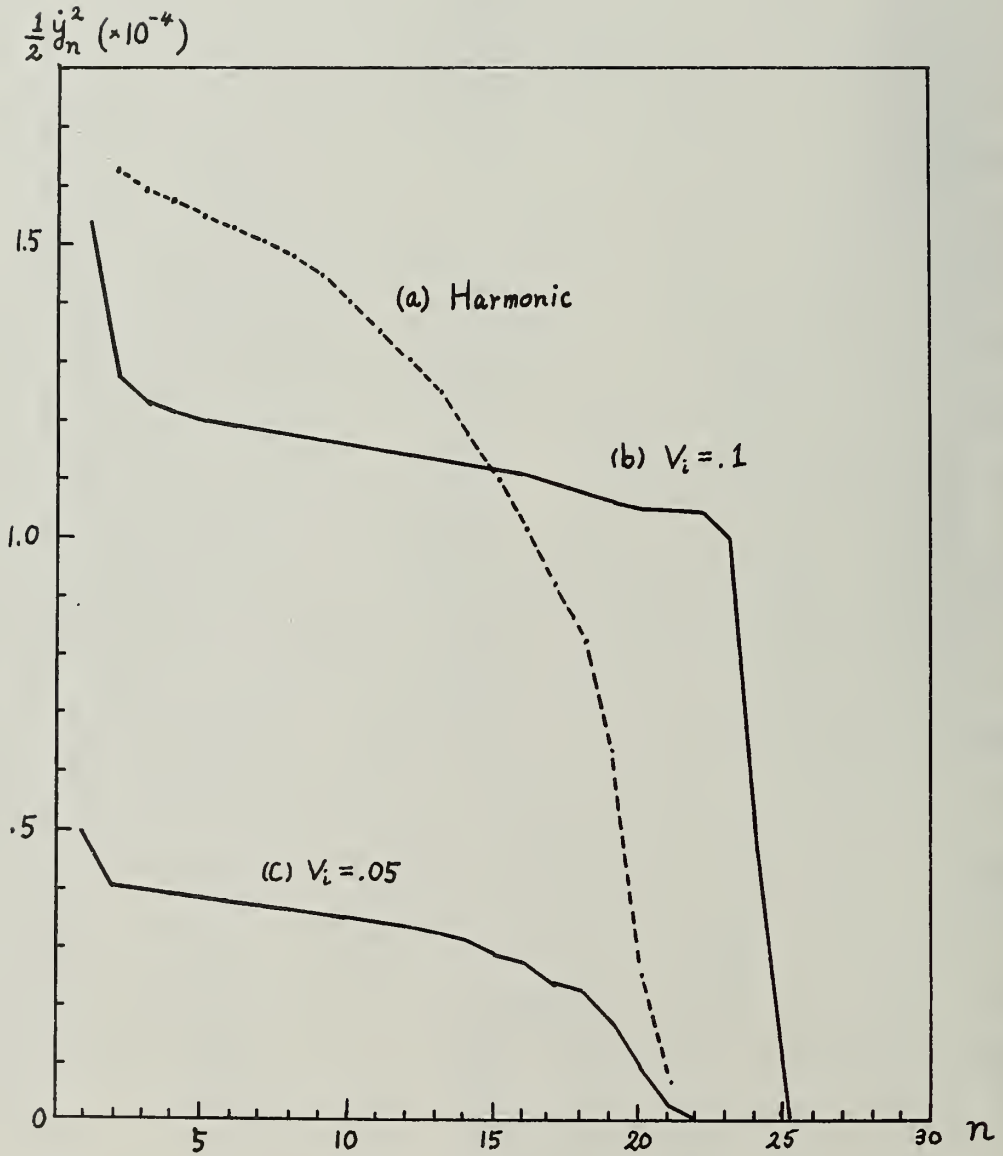


Fig. 5.17. Time averaged kinetic energy.

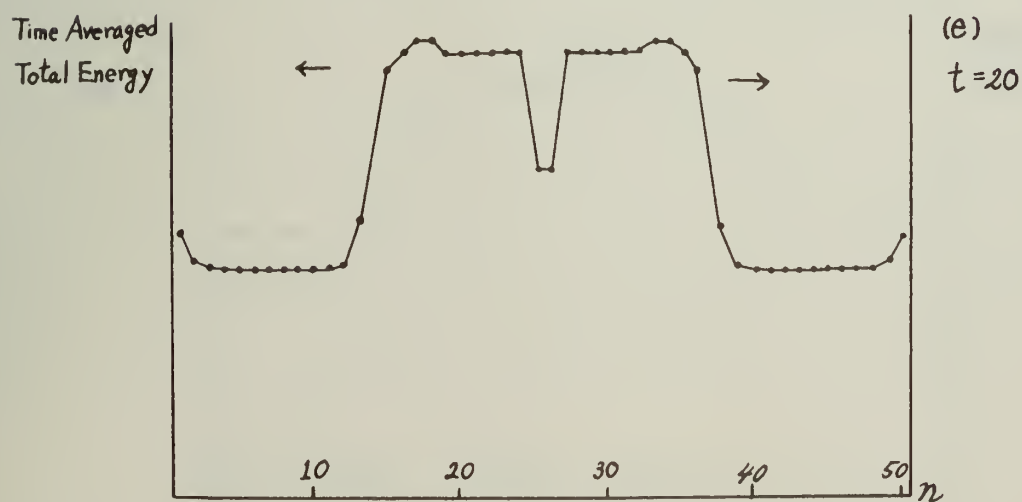
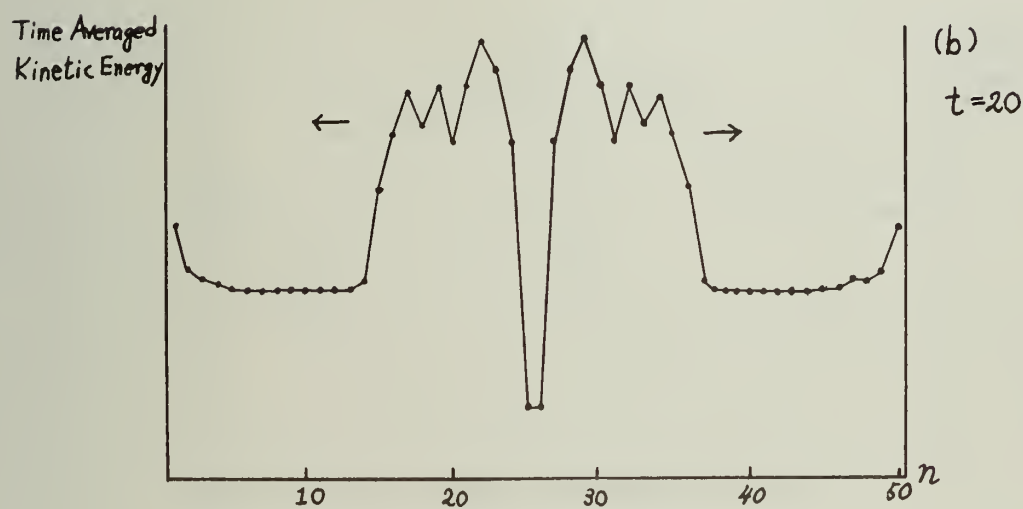
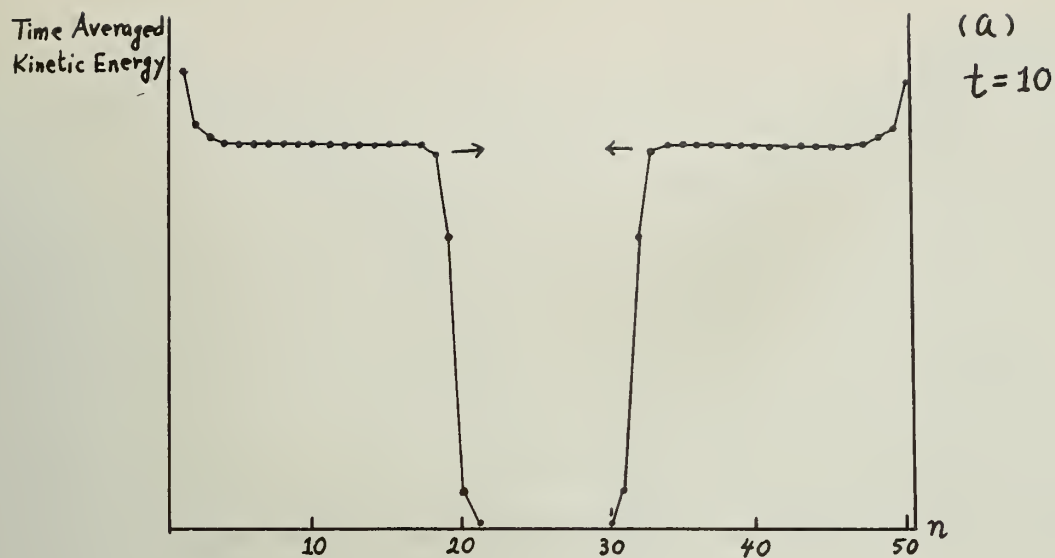


Fig. 5.18. Time averaged energy of each atom: JPW lattice (arbitrary unit).

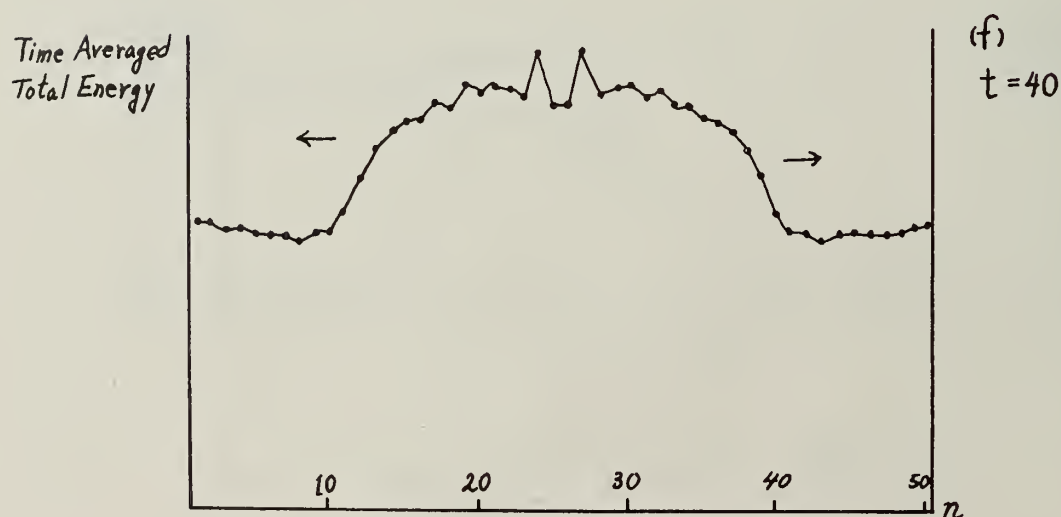
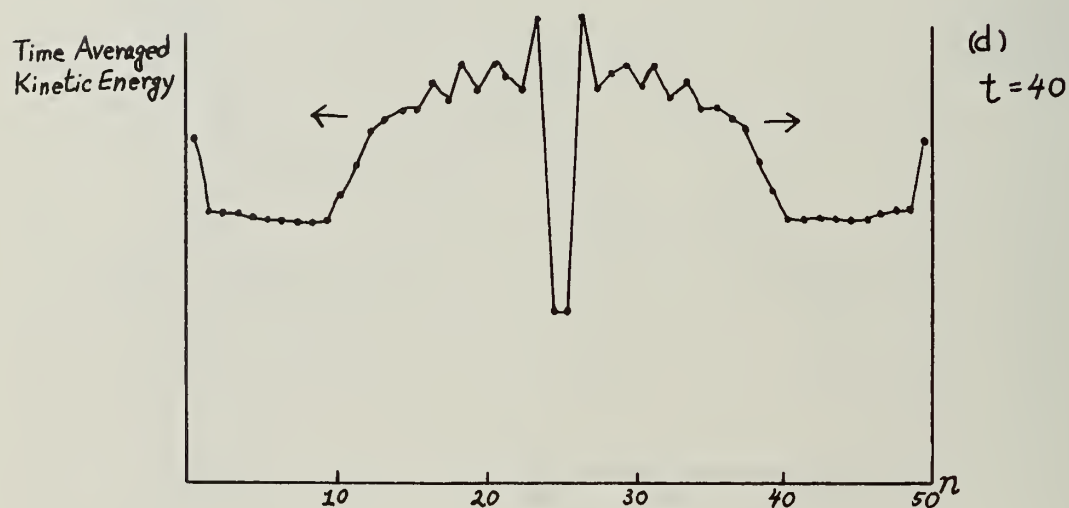
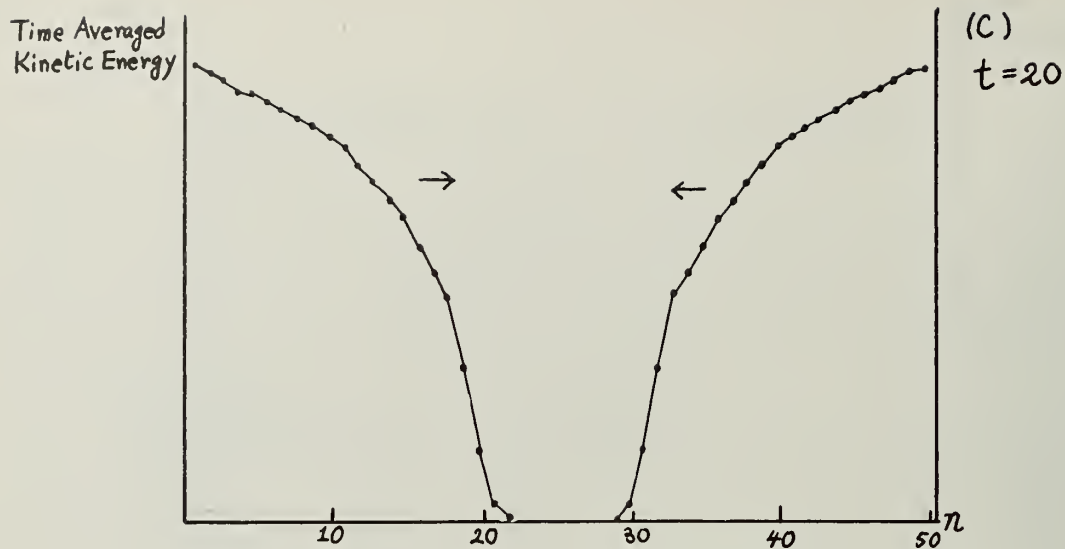


Fig. 5.18 (continued). Time averaged energy of each atom:
harmonic lattice (arbitrary unit).

equal probability. Therefore it will not leave any effect on the temperature distribution. We will use the kinetic temperature for the actual computation of the temperature distribution.

5.5 Piecewise Linear Force Function

As we discussed in Chapter 3 the piecewise linear force yields the solitary waves in the continuum approximation. We will show in this section that such solutions also exist in the anharmonic lattice (in the discrete system). We choose the force function as:

$$\begin{aligned} f(x) &= x & x > -b \\ f(x) &= 2x+b & x \leq -b \end{aligned} \quad (5.4)$$

It is obvious that the amplitude must exceed the threshold value b ; otherwise the wave motion would be pure harmonic.

The numerical results are given in Table 5.2 for various b and the initial velocities. A typical profile is given in Fig. 5.19. The two wave collision process was also examined for a typical value of V_i and b . Two solitary waves were verified to exist even after the collision. There was no phase shift nor energy left at the site of the collision.

5.6 Hard Sphere Plus Harmonic Force Function

The hard sphere plus harmonic force function first introduced by Northcote and Potts may be considered as a special case of §5.5.⁽¹³⁾ This model combines the harmonic lattice and a very strong nonlinearity, hence it is theoretically very convenient. We define the force function as:

$$\begin{aligned} f(x) &= x & x > -b \\ f(x) &= -\infty & x \leq -b \end{aligned}$$

where b is the collision distance (Fig. 5.20). Computationally the hard

Table 5.2
Solitary Waves in Piecewise Linear Force Model

b	V_i	Amp.	V
.01	2	.524	1.35
.05	2	.628	1.33
.1	2	.731	1.29
.2	2	.851	1.25
.4	2	.981	1.16
.6	2	1.025	1.086
.2	1	.491	1.167

b: break point

V_i : initial velocity

Amp.: amplitude of the solitary waves

V: propagation velocity

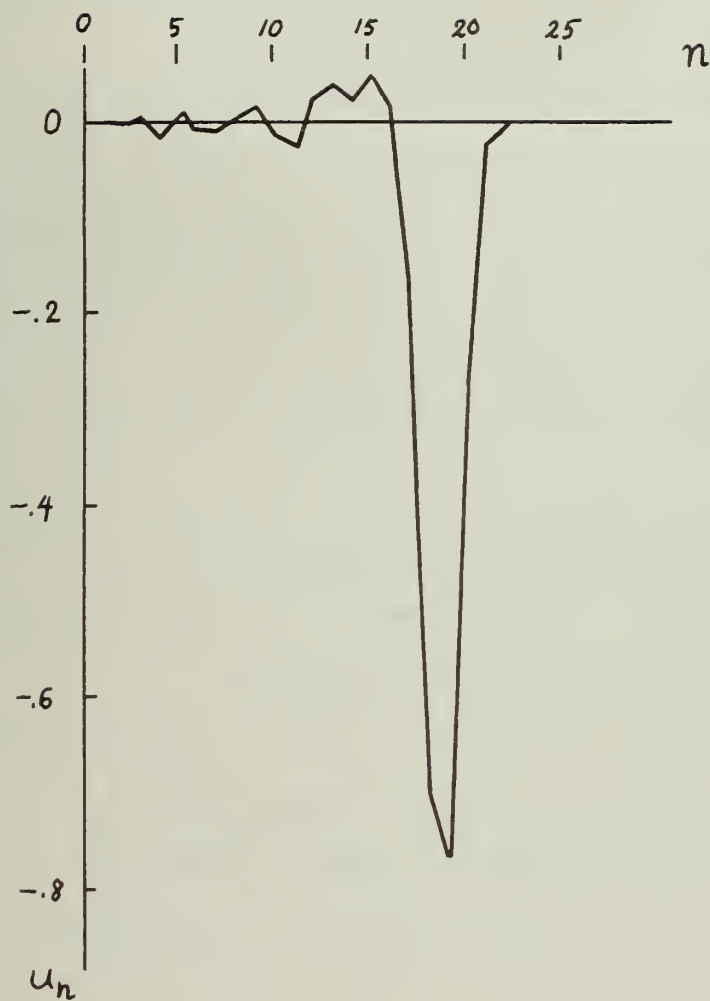


Fig. 5.19. Solitary wave in piecewise linear force lattice.

$$f(x) = x \quad x > -.2$$

$$f(x) = 2x + .4 \quad x \leq -.2$$

sphere type interaction can be realized by interchanging the velocities of two atoms when a collision takes place. We can obtain, on one hand, the harmonic lattice by increasing b , on the other hand, we can obtain the hard sphere gas model by letting b close to 0. In our numerical experiments we specifically chose $b = .5$. Judging from the results in the previous section we can expect the solitary wave solution in this model too. The numerical results are given in Table 5.3. A typical profile of the wave is also given in Fig. 5.21. We found that the solitary wave is quite stable, provided that the initial impulse is sufficiently large. Note that the wave motion is harmonic if the amplitude is less than b . For some critical values of amplitude the once formed solitary waves decay as they travel along.

We also examined the two wave collision process in this model. Fig. 5.22 shows an example. In this example, the initial velocities are .9 for both ends. The following facts are remarkable:

- (1) the energy is left at the site of a collision. The amount of this energy is considerably large ($\sim 4\%$);
- (2) both waves are advanced after the collision;
- (3) the velocities become smaller after the collision due to the loss of the energy.

It is notable that the energy loss in the collision process is large enough to affect the propagation velocity in this model. Presumably the same thing could happen in the JPW lattice; the nonlinear effect is too small to be noticeable. It is quite conceivable, however, that the solitary waves encounter many collisions in the thermal situation, if the lattice size is sufficiently large. Then the loss of the energy will be significant.

Table 5.3
Solitary Waves in Hard Sphere plus Harmonic Lattice

b	V_i	V	E_{sol}	E_{tail}	E_{col}^*	h
.5	.79 ^{**}	—	—	—	—	.025
.5	.80 ^{***}	1.19	—	—	—	.025
.5	.90	1.60	.4043	.0007	.01502	.025
.5	1.0	1.82	.4999	.0001	—	.025
.5	1.5	3.07	1.12500	$.2 \cdot 10^{-5}$	.00248	.025
.5	2.0	4.0	2.0000	$.5 \cdot 10^{-7}$	—	.025

* Collision of the two solitary waves of the same size.

** Decay at $n=12$.

*** Decay at $n=38$.

b: break point

V_i : initial velocity (initial energy = $.5 \cdot V_i^2$)

V: propagation velocity

E_{sol} : energy in the solitary wave part

E_{tail} : energy in the tail

E_{col} : energy loss at a collision

h: integration step

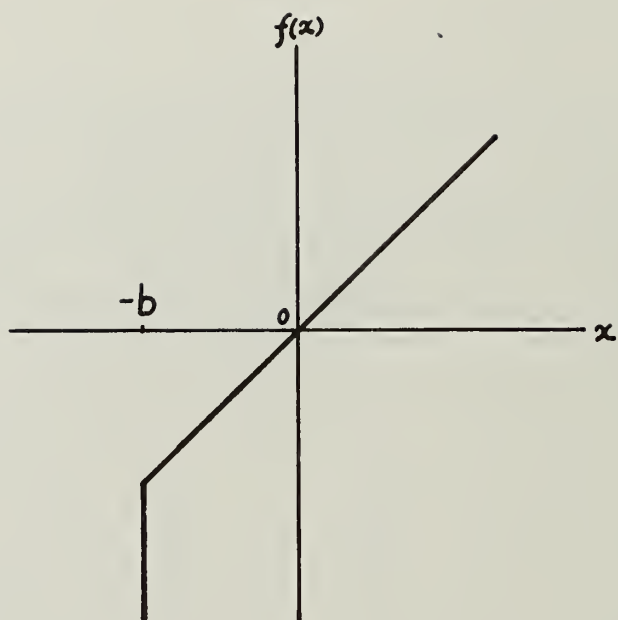


Fig. 5.20. Hard sphere plus harmonic force.

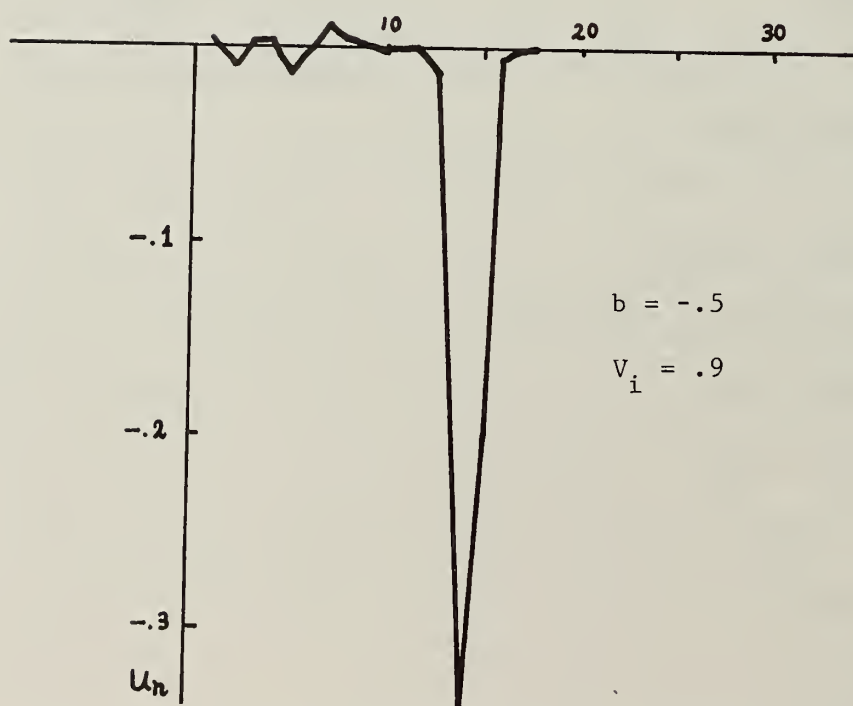


Fig. 5.21. Solitary wave in hard sphere plus harmonic force lattice.

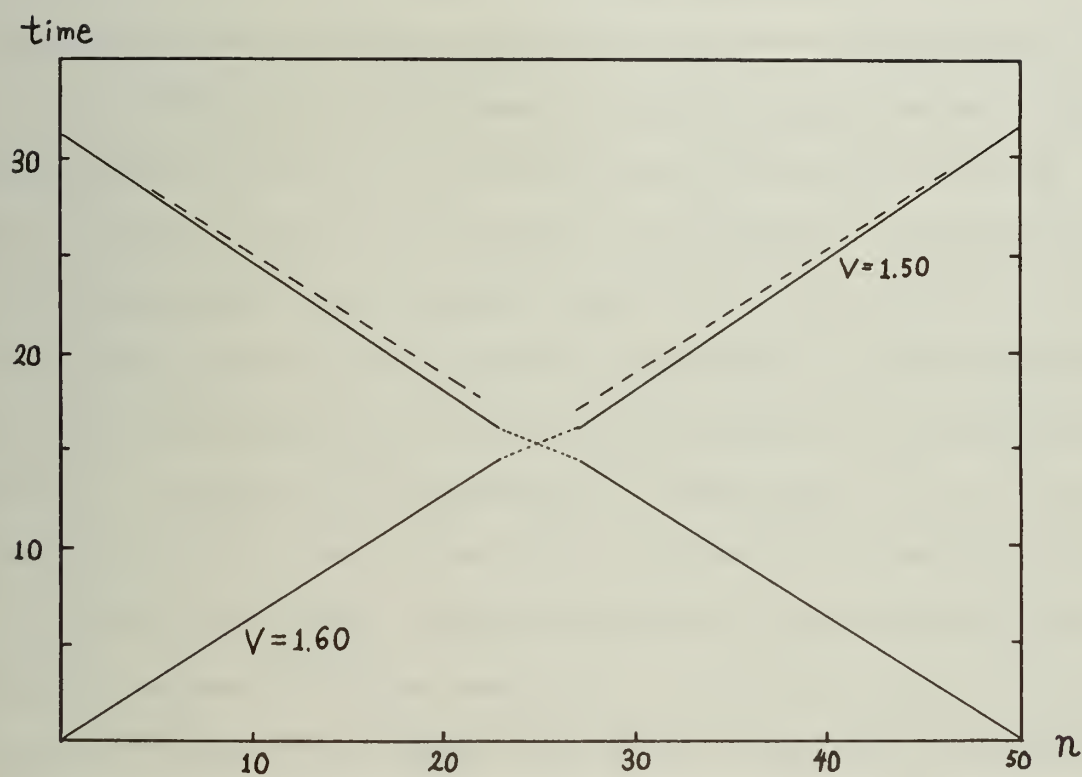


Fig. 5.22. Head on collision for hard sphere plus harmonic force model.

CHAPTER 6. HEAT CONDUCTION PROBLEM IN ANHARMONIC LATTICES AND ITS PHENOMENOLOGICAL INTERPRETATION

We will consider the heat conduction problem in this chapter. Our main purpose is to investigate the applicability of the idea of the solitary waves to this problem. As we discussed in the previous chapter the JPW lattice and the hardsphere plus harmonic lattice (to be called H+H lattice) both have the solitary wave solutions. The heat conduction problem has been numerically considered by several authors and the temperature gradient has been observed in both types of lattices. ^{(21), (44)}

We can obtain a better insight into this problem by locating these two types of lattices between two extreme cases; the harmonic lattice, the JPW lattice, the H+H lattice and the hard sphere lattice. They are put in the increasing order of nonlinearity, in a sense. The last model will need some introduction. In this model each atom of the lattice can travel freely in the interatomic space until it collides with its neighbors. The collision is assumed to be elastic as is the case for H+H lattice. Since the velocities of two atoms are exchanged in each collision, the energy can propagate through the lattice as if it were carried by one atom which passes through others without any interaction. Therefore, if this lattice interacts with two heat reservoirs of different temperatures, the internal temperature distribution will be uniform, although there is a heat flux from the high temperature side to the low temperature side. This model is equivalent to Knudsen gas model, in which each atom literally propagates from one reservoir to another without collision. ⁽⁴⁵⁾ The harmonic lattice, on the other hand, also has the same thermal characteristics as the hard sphere lattice. In this case each Fourier component (or the normal mode) carries the energy independently of other modes at its group velocity, hence

there is no temperature gradient. We also derived the same tendency for the semi-infinite harmonic lattice (§2.6). It is interesting to note this conceptual resemblance in these two models. If we are to consider the solitary waves as the media which carry the heat in the JPW lattice and also in the H+H lattice, we encounter a serious paradox: the solitary waves are conceptually identical to the individual atoms in the hard sphere lattice or the Fourier components in the harmonic lattice. Hence there would be no temperature gradient. This, of course, is a contradiction to the observed temperature gradient both in numerical computation and in the real crystals! We will propose in this chapter a phenomenological theory to solve this apparent paradox. Our discussion will be mainly qualitative due to the following drawback in the present stage:

- (1) No concrete theory has been established for the solitary waves in the JPW lattice. Therefore we must use the empirical relations such as those obtained in Chapter 5.
- (2) The stochastic nature of the present problem greatly limits the accuracy of the solutions due to the fluctuation therein. A tremendous amount of computation time is required to obtain the numerical results which are accurate enough for the quantitative discussions.

In the first part of this chapter we will analyze the numerical results for our model lattice ($N=50$, JPW type force function). In §6.1 we will consider the cooling process. The heat reservoirs have zero temperature, so that they work as heat sinks. We will compare our heat reservoirs and the viscous type heat sink introduced by Nakazawa.⁽²⁰⁾ In §6.2 we will adversely consider the heating process of a cold lattice. Only the anharmonic lattice

will be treated here since our purpose is to observe the formation of the temperature gradient. In §6.3 we will consider the heat conduction process which we briefly introduced in Chapter 1. We will compare different boundary conditions. In §6.4 we will interpret the heat conduction phenomena in terms of the solitary waves. In §6.5 we will discuss H+H model and we will imply the importance of the collision process with regard to the formation of the temperature gradient.

6.1 Cooling Process of Anharmonic Lattices

We computed the residual energy in the lattice when two reservoirs have zero temperature to demonstrate that our heat reservoirs actually have viscous effect. We also examined the viscous type heat reservoir used by Nakazawa for comparison (§4.3). In the latter case the end atoms lose their energy no matter where they are located (§4.3). The results are in Fig. 6.1. The curve I corresponds to our model heat reservoirs and the curve II corresponds to the viscous type. The initial conditions are the same for both cases. The energy loss is faster in the latter case due to the continuous interaction. Our model may be described as having the infinite viscosity inside the reservoirs but none outside.

6.2 Heating Process of Anharmonic Lattices

The purpose of this numerical experiment is to observe how the temperature behaves in the early stage of the heating. The only difference between this experiment and those in the next section is the initial condition. The temperature distributions are given in Fig. 6.2. The reservoirs have the temperatures .02 and .01, respectively. At $t=0$ two solitary waves were produced. Fig. 6.2a, for example, is the temperature distribution at $t=50$.

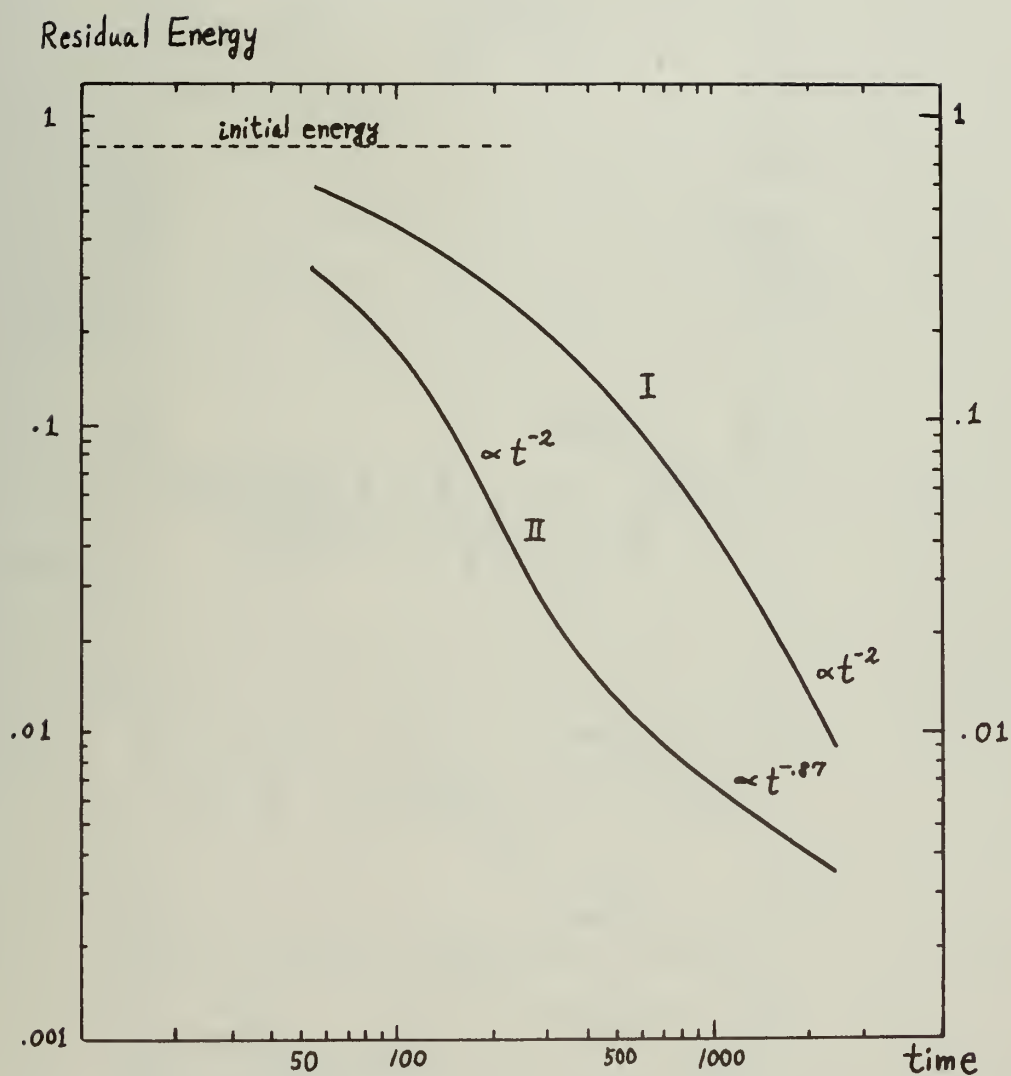


Fig. 6.1. Cooling process

Curve I : Impact type reservoirs

Curve II: Viscous type reservoirs ($\mu_1 = \mu_N = -.5$).

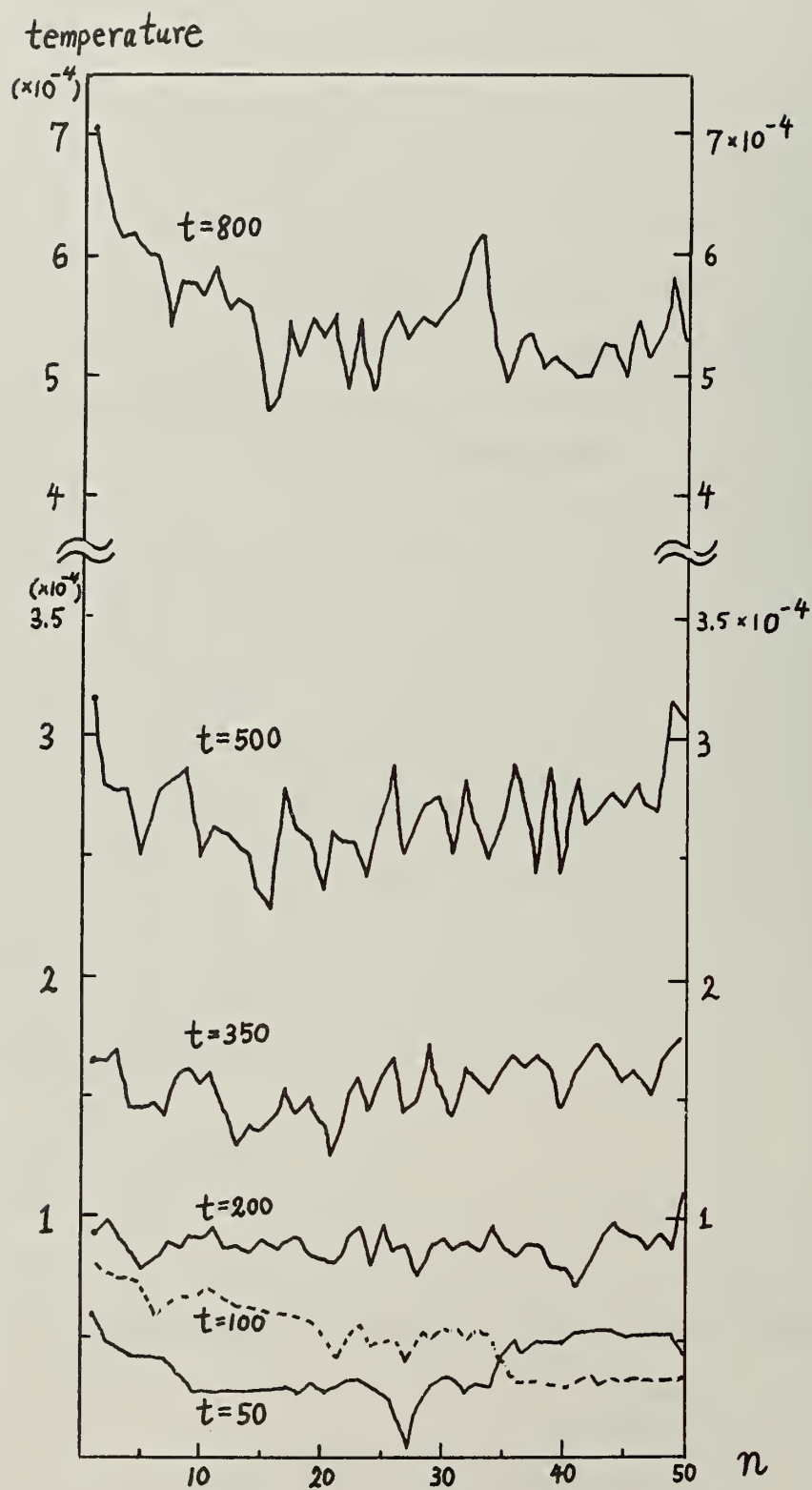


Fig. 6.2. Temperature distributions in warming process.

By this time two solitary waves have interacted with the reservoirs and they have been reflected. Their locations are at $n=8$ and $n=35$. We can clearly see the individual contributions of the solitary waves and the tails to the temperature distribution. There is also a temperature hole at $n=27$, indicating a collision which occurred there. As time goes on, more interaction with the reservoirs takes place and the temperature rises. Sometimes the temperature has a positive gradient, but this is a temporary effect caused by the large amplitude solitary waves which happened to be near the low temperature end. Such an irregularity will be removed with time. The effect of the temperature holes also disappears with time.

The numerical experiment in this section is preliminary to those in the next section, where we will consider the long time behavior of the lattices.

6.3 Heat Flux and Temperature Distribution under Different Boundary Conditions

In this section we consider the heat conduction problem. We performed numerical experiments with different boundary conditions. As we described in Chapter 4, the location of the end atoms were checked at every m integration steps, where the integration step is .05. Specifically, $m=1, 5$ and 20 . Initially the atoms were given random velocities sampled from the probability density (1.4) with $T=.5(T_1+T_2)$, where T_1 is the temperature of the left reservoir and T_2 is the temperature of the right reservoir. Specifically, $T_1 = .02$ and $T_2 = .01$. We ran one case with $T_1 = .012$ and $T_2 = .008$. The latter case was also chosen by JPW. In some cases the atoms also had the initial disturbances in the displacement too. We also ran a harmonic case to single out the qualitative effects of nonlinearity.

Due to the limitation of the available computation time, the maximum simulation time was 6000 dimensionless seconds and in most cases 3000 seconds. Therefore the results obtained by JPW are superior to ours. The results are in Table 6.1. The accumulated flux and the temperature distributions are also given in Fig. 6.3 and Fig. 6.4 for two typical cases.

We will summarize the important facts of our results in the following;

(1) The heat flux becomes stationary at an early stage. We calculated the heat flux from the data on the accumulated flux by the least square fitting after the temperature of the 25th atom becomes steady. In the long run the flux thus obtained will match (accumulated flux)/(simulation time). The fact that the flux is immune to the temperature fluctuation (to be discussed later) seems to support the idea of the solitary waves as the heat carriers, since the solitary waves are also immune to the background disturbances. We can consider that the data on the flux is quite reliable.

(2) There is a tendency for the heat flux $\bar{J}$ to increase with m .

(3) The temperature gradient is a very fluctuating quantity. It is very difficult to obtain reliable data. JPW also reported this difficulty.

There is a tendency, however, for the temperature gradient to increase with m .

(4) The empirical thermal conductivity $k_T = \bar{J}/(-\nabla T)$ is dependent on the boundary condition. Since the fluctuation of the temperature gradient is large, we cannot make quantitative analysis on this.

(5) We recorded the entire history of the interaction between the lattice and the reservoirs; that is, time of interaction, incoming velocities and outgoing velocities. From these data we could fairly well identify the propagation of the solitary waves of large amplitudes. More precisely, for

Table 6.1
Numerical Experiments on Heat Conduction Problem

Exp. No.	m	time	C_1	C_r	$\bar{J}(10^{-3})$	$-\nabla T(10^{-5})$	κ_T	t_J	T_1/T_2
1	1	3000	230	267	1.15	1.56	73.7	1600	.02/.01
2	1	6000	221	267	1.06	1.78	59.6	2000	.02/.01
3	5	3000	246	325	1.25	4.4	28.4	1600	.02/.01
4	5	3000	245	315	1.23	3.76	32.7	1600	.02/.01
5	5	4000	234	294	1.19	3.94	30.2	2100	.02/.01
6	20	2000	262	331	2.00	8.90	22.5	1000	.02/.01
7	1	3000	219	269	.434	1.28	34	1600	.012/.008

Note:

m: boundary crossing of the end atoms is checked at every m integration steps.

time: maximum simulation time.

C_1, C_r : collision frequencies at the boundaries (per 1000 sec).

$\bar{J}$: averaged heat flux.

∇T : temperature gradient.

κ_T : empirical thermal conductivity ($-\bar{J}/\nabla T$).

t_J : the time at which T_{25} becomes stationary.

T_1/T_2 : the temperature of the reservoirs.

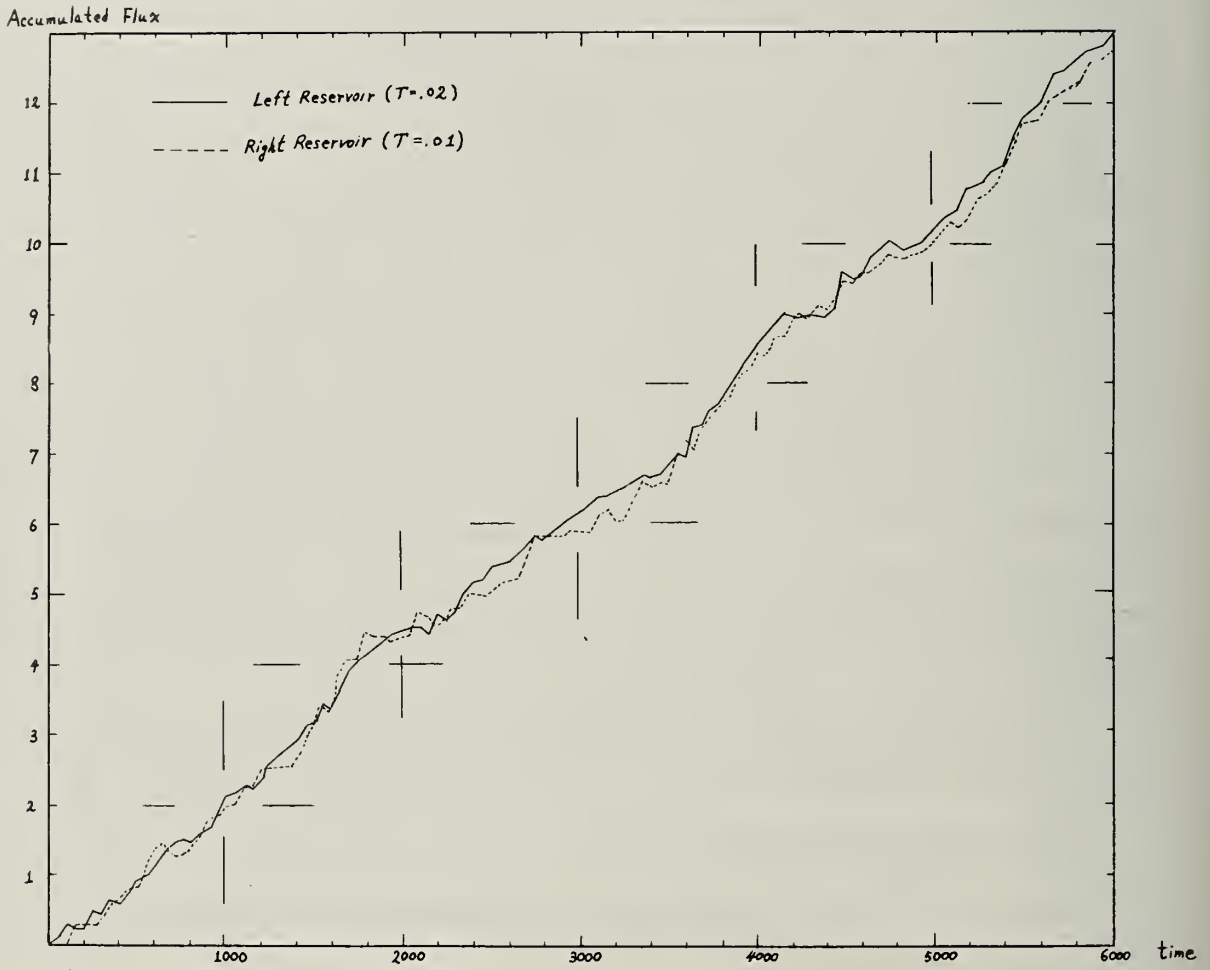
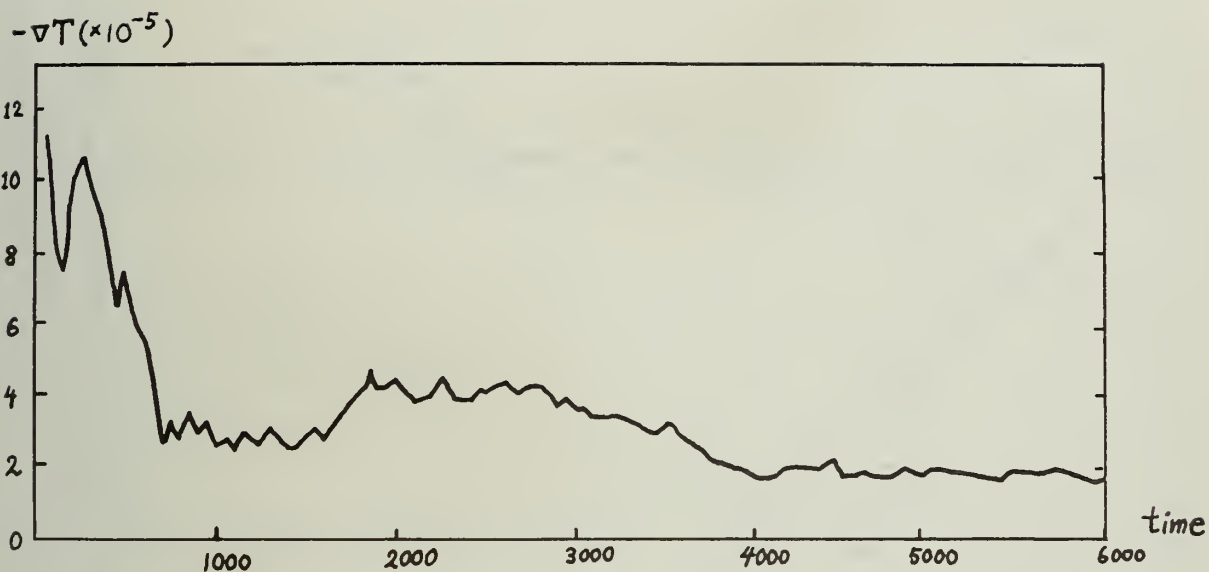
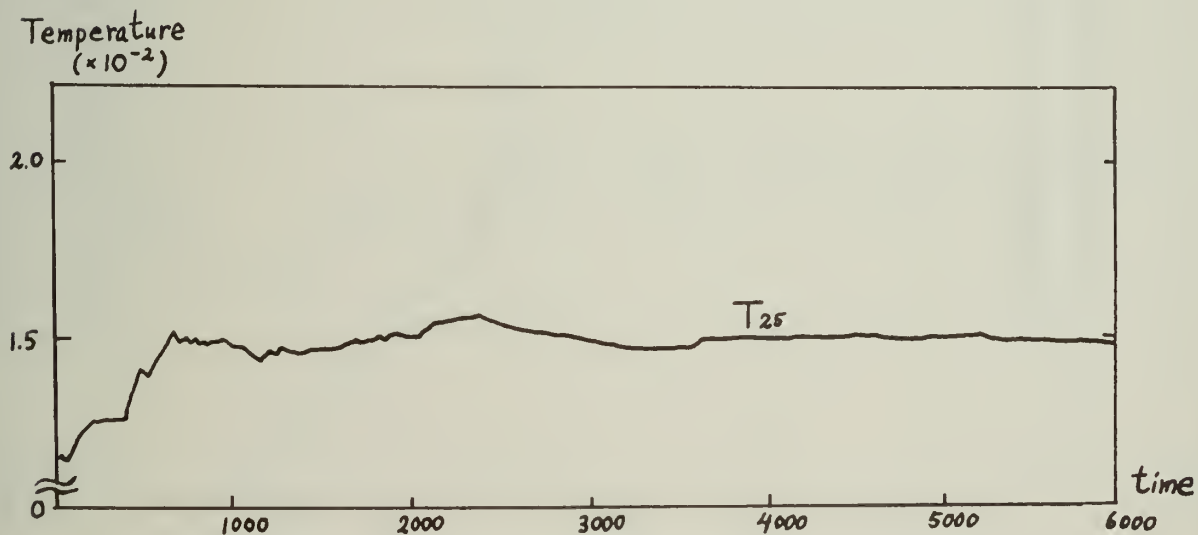


Fig. 6.3a. Accumulated flux (Data No. 2).



(b) Temperature gradient



(c) Temperature of 25th atom

Fig. 6.3 (continued). Internal temperature gradient and T_{25} (Data No. 2).

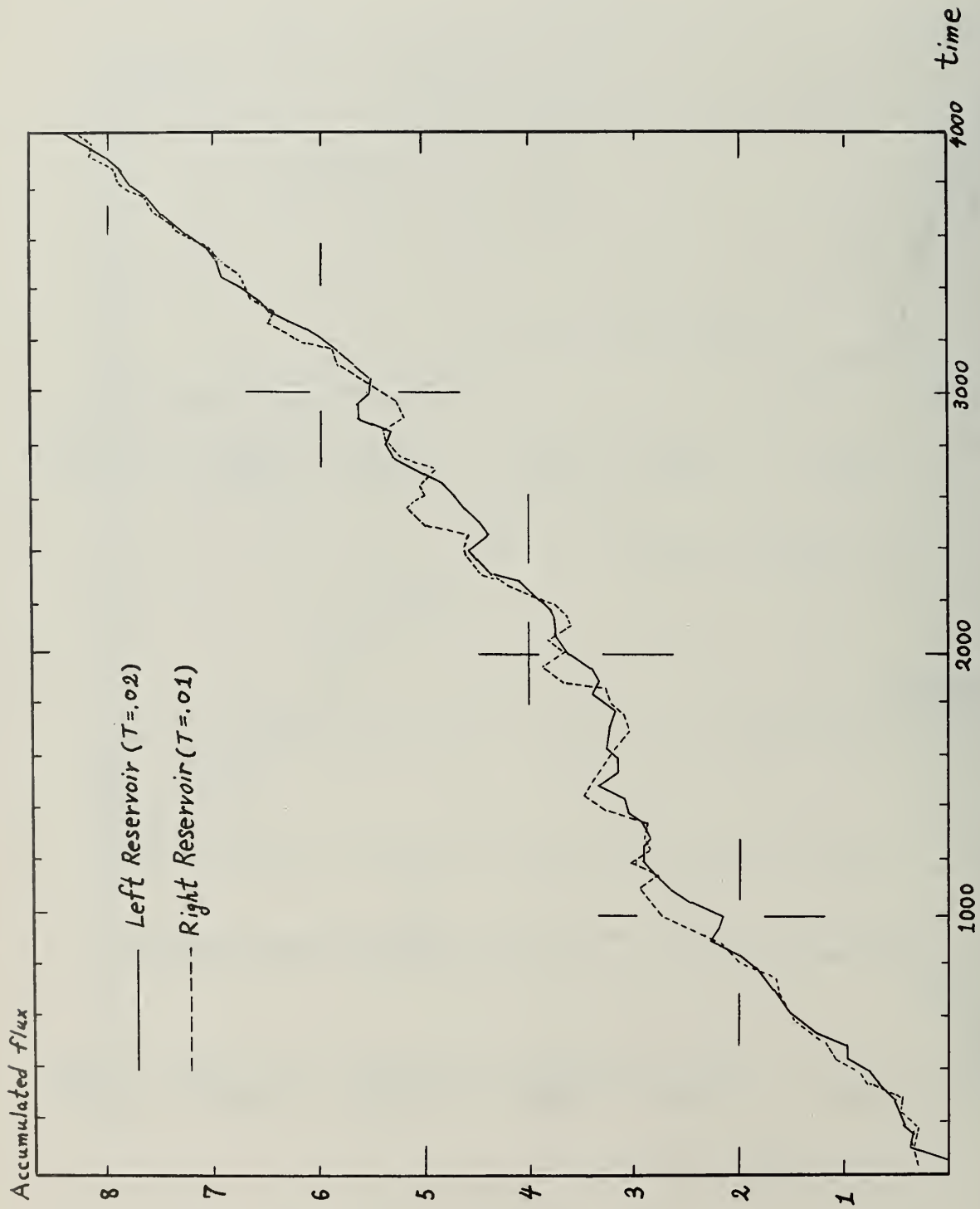
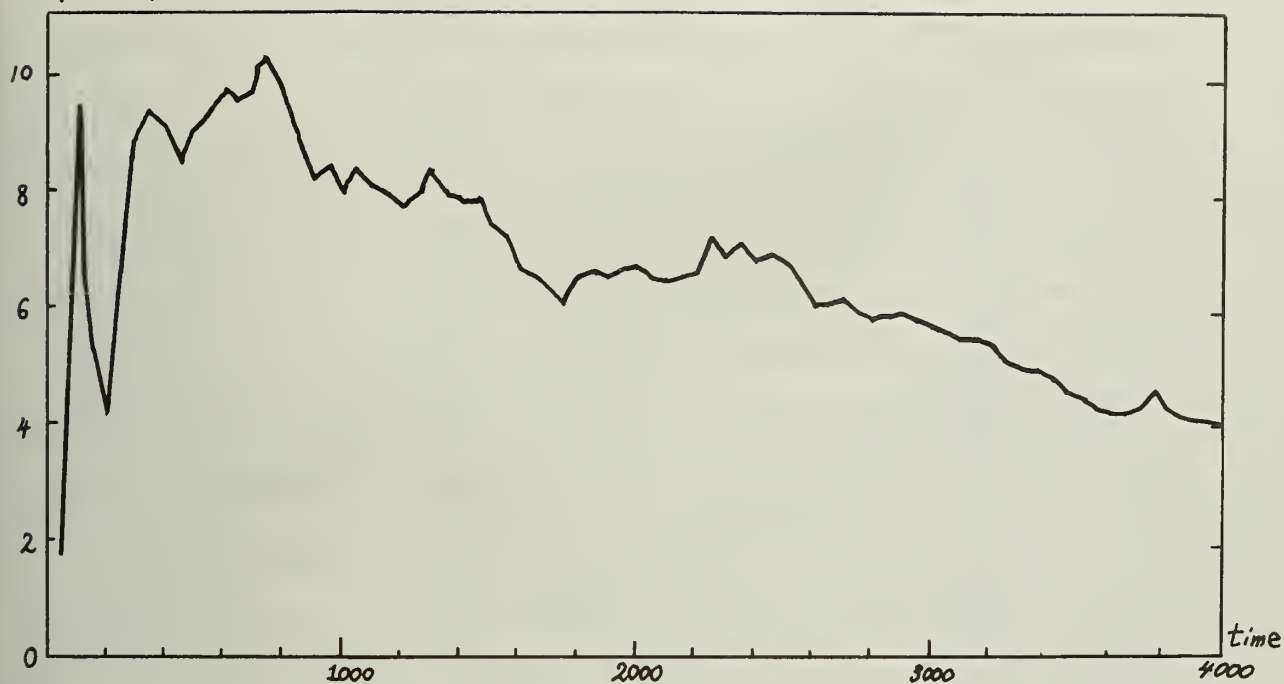
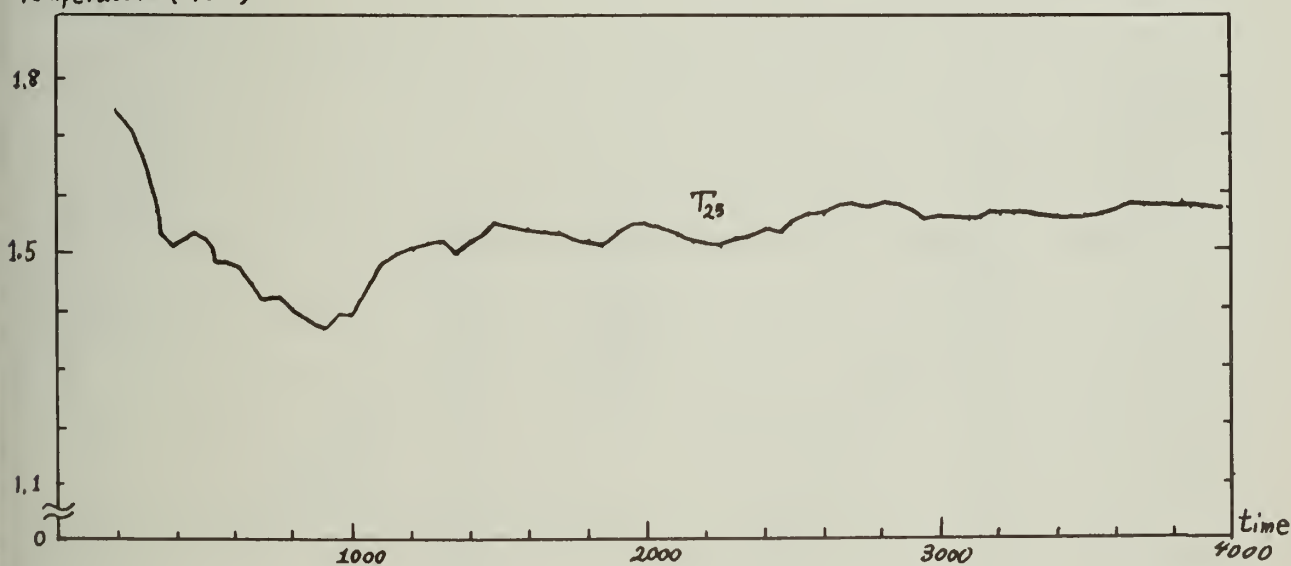


Fig. 6.43. Accumulated flux (Data No. 5).

$-\nabla T (\times 10^{-5})$


(b) Temperature gradient

 Temperature ($\times 10^{-2}$)


(c) Temperature of 25th atom

Fig. 5.4 (continued). Internal temperature gradient and T_{25} (Data No. 5).

a velocity v_1 given to the atom $n=1$ at $t=t_1$ we can find a corresponding interaction in the other end of the lattice at $t=t_2$, where t_2-t_1 is close to the time it takes a solitary wave to cross the lattice with the initial velocity v_2 . We used the initial velocity vs propagation velocity relation in Fig. 5.6. We also found that the interaction time is not distributed uniformly but more dense when a solitary waves arrive at the end of lattice.

It is clear that the solitary waves introduce interaction with the reservoirs.

(6) Histograms of the velocities of the end atoms, at the time of interaction with the reservoirs were obtained from the above data. They are in Fig. 6.5. The distributions after the interactions are merely the sampling from the probability density function (1.4) with $T=.02$ for $n=1$ and $T=.01$ for $n=50$, respectively. We could not determine, however, the nature of the distributions for the incoming velocities due to fluctuation. This difficulty was also reported by JPW.

(7) The collision frequency is higher on the low temperature side. This difference is necessary to retain the lattice between the two reservoirs. In other words the total momentum of the lattice is balanced to zero in the time average. Consequently the pressure is the same on both sides.⁽²¹⁾

(8) The temperature distribution showed a periodic structure. This phenomenon was also observed by JPW and by Helleman.⁽⁴⁴⁾ (Fig. 6.6.)

(9) The heat flux $\bar{J}$ is considerably lower in the harmonic lattice. This result was also reported by JPW and by Helleman. Since the collision frequency is also low in the harmonic lattice we cannot single out the nonlinear effect from this result. We can explain the low collision frequency in the harmonic lattice as follows; firstly the anharmonic lattice is stiffer than the harmonic lattice, therefore the "sloshing" effect of the lattice is less

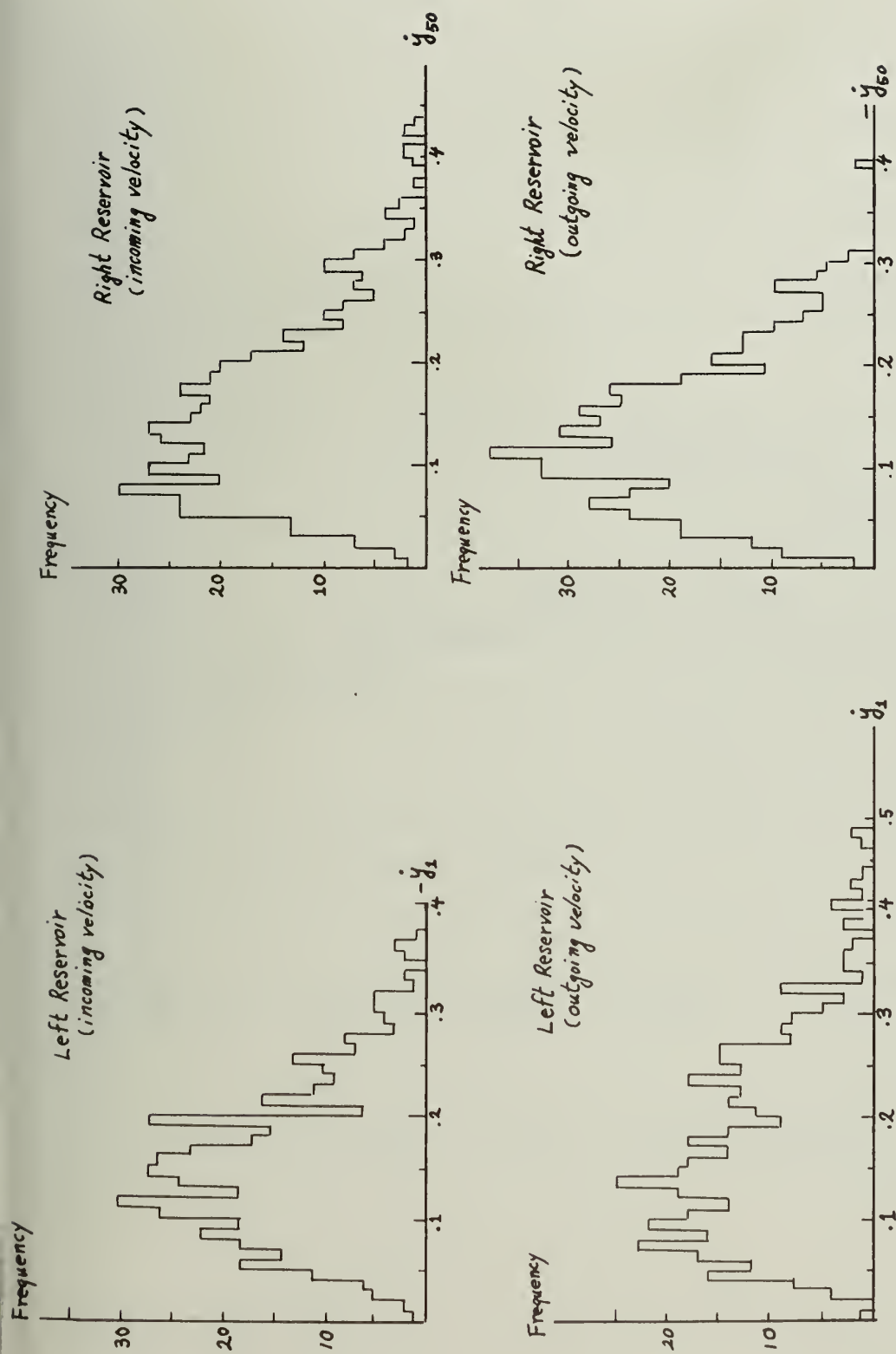


Fig. 6.5. Histograms of velocities of end atoms (Data No. 2 $t=0 \sim 2000$ sec).

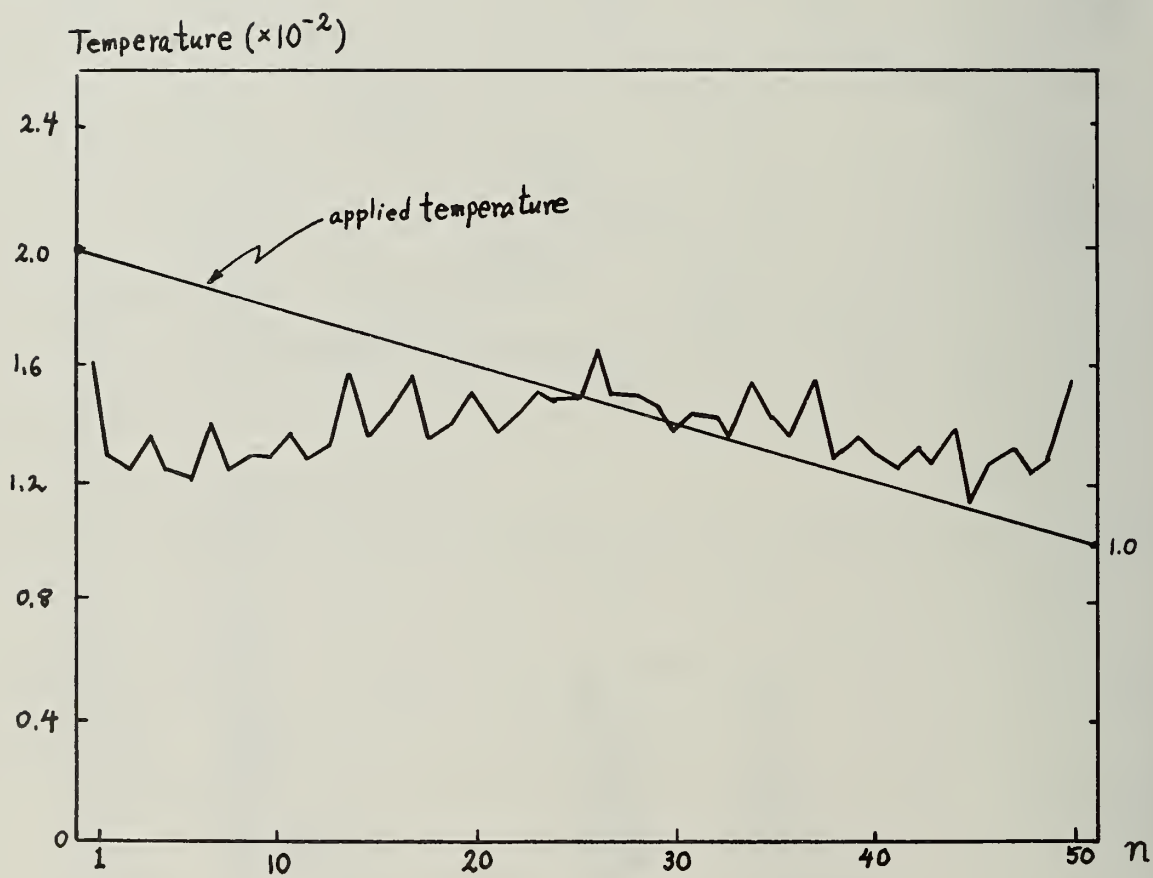


Fig. 6.6. Periodic behavior of internal temperature distribution for harmonic lattice.

important in the anharmonic lattice. Secondly the solitary waves propagate faster than the sound velocity, resulting in more collisions per unit time. From the above reasons we can say that the thermal contact is better in the anharmonic lattice. In the present scheme of the interaction between the lattice and the reservoirs the heat flux seems to be limited by the boundary effects rather than by the properties of the lattice itself. Especially the "sloshing" effect of the lattice is not likely to happen in the real crystals.

6.4 Phenomenological Interpretation of Heat Conduction in JPW Lattice

We consider the heat conduction problem in the JPW lattice in terms of the solitary waves and the tails. First we should recall that the interaction between the lattice and the reservoirs produce either the solitary wave and the tail (when V_i is sufficiently large) or a wave packet which does not yield the solitary wave and the tail within the limit of the lattice size (when V_i is small) (§5.1). The numerical results in the previous section as well as in Chapter 5 strongly indicate that the solitary wave carries the major portion of the heat. Because of the high concentration of the energy and the high propagation velocity, the energy is transferred very efficiently (§5.1, §5.2). The solitary wave is not absorbed completely in the reservoirs but partially reflected (§5.2). At the same time, new solitary waves are created due to the interactions induced by the incoming solitary wave. Therefore the solitary wave also works as the "exciter". Because of the high propagation velocity, the collision frequency between the lattice and the reservoirs is considerably increased ((9), §6.3). An important fact is that the momentum balance of the entire lattice ((7), §6.3) is maintained chiefly by the "catch ball" of the solitary waves between the two reservoirs.

The tail (including the wave packets for the low initial velocities) is characterized by dispersiveness, low energy and low propagation velocity. Its contribution to the heat flux is not significant, but the individual tail gives a decreasing contribution to the temperature in the direction in which it propagates (§5.4). We should note that there is a big difference between the waves in the harmonic lattice and the tails in the anharmonic lattice, although both waves are harmonic. In the former case, the harmonic waves are responsible for the momentum balance of the lattice as well as for the heat flux, whereas the tails are responsible for none of them in the latter case. In other words, there is a constant (small) flow of the tails from each reservoir in the anharmonic lattice, the flow rate being determined by the traffic of the solitary waves. We can expect that the unbalanced flows in two directions due to the temperature difference will result in some gradient from the high temperature to the low temperature side. This is what we propose to solve the paradox which we stated in the beginning of this chapter, since both the collision process and the interaction between the solitary waves and the disturbances do not seem to be significant in our model lattice. Unfortunately we do not have enough numerical evidence as yet to support this proposition quantitatively.

The disturbances in the lattice are the collection of dispersed tails. Since the tail loses its coherency as it propagates, the disturbances are quite incoherent and do not contribute to the heat flux. The energy of the disturbances does not increase indefinitely but is maintained at a certain level on the average due to the interaction with the reservoirs.

The heat flux and the temperature gradient are related to each other through the nonlinear coefficients; the propagation velocity, fraction of

the energy in the solitary waves and the stiffness of the lattice are all dependent on the nonlinear coefficients.

The effects of the boundary conditions on such quantities as the heat flux, the temperature gradient and the thermal conductivity are not clear. Presumably the energy is more efficiently exchanged at the reservoirs if the end atoms have more freedom (i.e. m is large). Therefore we can expect higher flux in such cases.

At any rate the dependency of the thermal conductivity on the boundary conditions implies that this quantity is not intrinsic to the lattice.

Finally, we will summarize the results of this section.

- (1) The solitary waves carry the major portion of the heat.
- (2) The solitary waves considerably increase the collision frequency with the reservoirs, due to high propagation velocity.
- (3) The solitary waves also maintain the momentum balance of the lattice.
- (4) The tails are one possible source of the temperature gradient in the JPW lattice.

For other possibilities of the source of the temperature gradient, refer to the next section.

6.5 Hard Sphere Plus Harmonic Type Model and Other Possibilities of the Temperature Gradient

As we discussed in the previous section, the JPW lattice has the characteristics of Knudsen type model. We next consider the H+H type model. Helleman investigated the heat conduction problem in this model and discovered that the temperature gradient becomes more obvious than in JPW lattice.⁽⁴⁴⁾ We showed in §5.6 that H+H type lattice also has the solitary wave solution and we discovered that a non-negligible amount of the energy

was lost from the solitary waves in the two wave collision. From these results we can consider the collision process as very important in the strongly anharmonic lattices. Namely, the solitary waves lose significant amount of energy as they collide with other solitary waves. In this picture the relation between the heat flux and the temperature gradient becomes inherent to the lattice. Another possibility is the interaction between the solitary waves and the disturbances. In the JPW lattice the effect of the disturbances is not important. But if we increase the number of the atoms enormously, such effect may not be negligible any more. In this case, too, the solitary waves will decay as they propagate through the lattice. No research has been done in this area, however. We will need a very high speed computer of the Illiac IV class to perform numerical experiments with super large-sized lattice.

CHAPTER 7. CONCLUSION

In this thesis we considered the properties of the solitary waves both analytically and computationally. In the first approach we introduced the piecewise linear function model, by which most of the special characteristics of the solitary wave solution and also the periodic solutions can be explained with the elementary functions. As for the second approach, we performed numerical experiments on the anharmonic lattice introduced by Jackson, Pasta and Waters. We discovered that the impulse applied to the end atom of the lattice produces the solitary wave very efficiently. By this method we performed various kinds of experiments as to the properties of the solitary waves. One remarkable thing is that the solitary waves thus created lose their energy in the collision process. This has never been reported. Although the amount of loss at each collision is very small, this fact indicates the picture of the decaying solitary waves in the anharmonic crystals. We could also show that the piecewise linear function model and the hard sphere plus harmonic type model also have the solitary wave solutions.

Our numerical results were applied to interpret the heat conduction phenomena. Numerically we could show that the major part of the heat flux is carried by the solitary waves. The origin of the temperature gradient is still unclear, but the dispersive wave packets which are created with the solitary waves while the lattice interacts with the heat reservoirs might be a possible source. The collision process and the interaction with the disturbances seem to be negligible in our model lattice. Our numerical results indicate that the heat flow in our model lattice is near Knudsen

type. It is conjectured that the thermal conductivity will become the intrinsic quantity by increasing the lattice size considerably.

Finally, we mention that the numerical integration method due to Nyström was found to be superior to the classical Runge-Kutta type integration method.

APPENDIX A SOME PROPERTIES OF TCHEHYCHEFF'S ORTHOGONAL FUNCTIONS

Tchehycheff's equation

$$(1-w^2) \frac{d^2 y}{dw^2} - w \frac{dy}{dw} + n^2 y = 0 \quad (\text{A.1})$$

has two solutions^{(25), (26)}:

$$y_1 = T_n(w) = \cos(\text{narccos } w) \quad \text{first kind} \quad (\text{A.2})$$

and

$$y_2 = U_n(w) = \sin(\text{narccos } w) \quad \text{second kind} . \quad (\text{A.3})$$

Note that the above solutions differ from the usual solutions by the factor 2^{n-1} (according to van der Pol⁽⁴⁵⁾). $T_n(w)$ is a polynomial of n^{th} order, whereas $U_n(w)$ is the product of $\sqrt{1-w^2}$ and a polynomial of $n-1^{\text{st}}$ order.

Explicit solutions are given as follows for $n = 0 \sim 4$:

$T_0(w) = 1$	$U_0(w) = 0$
$T_1(w) = w$	$U_1(w) = \sqrt{1-w^2}$
$T_2(w) = 2w^2 - 1$	$U_2(w) = 2w\sqrt{1-w^2}$
$T_3(w) = 4w^3 - 3w$	$U_3(w) = (4w^2 - 1)\sqrt{1-w^2}$
$T_4(w) = 8w^4 - 8w^2 + 1$	$U_4(w) = (8w^3 - 4w)\sqrt{1-w^2} .$

Note that $T_n(w)$ is an even function of w when n is even, whereas $U_n(w)$ is an odd function of w when n is even.

Since $\arcsin w = \frac{\pi}{2} - \arccos w$,

$$\begin{aligned} \cos[(2n+1)\arcsin w] &= \cos[(n+\frac{1}{2})\pi - (2n+1)\arccos w] \\ &= (-1)^n \sin[(2n+1)\arccos w] \\ &= (-1)^n U_{2n+1}(w) . \end{aligned} \quad (\text{A.4})$$

The relation between Bessel functions and Tchebycheff's polynomials is best explained by using Hansen's integral representation for the Bessel function of integer order⁽²⁵⁾:

$$J_n(t) = \frac{i^{-n}}{\pi} \int_0^{\pi} e^{it \cos \theta} \cos n \theta \, d\theta . \quad (\text{A.5})$$

By introducing a new variable $w = \cos \theta$,

$$\begin{aligned} J_n(t) &= \frac{i^{-n}}{\pi} \int_{-1}^1 e^{itw} \cos[n \cos^{-1} w] (-\sin \theta)^{-1} dw \\ &= \frac{i^{-n}}{\pi} \int_{-1}^1 \frac{T_n(w)}{\sqrt{1-w^2}} e^{iwt} dw . \end{aligned} \quad (\text{A.6})$$

The above relation shows that the Bessel function has no higher frequency components than $w^2 > 1$. This corresponds to the fact that we are dealing with the low pass filter (§2.1).

Furthermore,

$$\begin{aligned} \frac{J_n(t)}{t} &= \frac{1}{2n} (J_{n+1}(t) + J_{n-1}(t)) \\ &= \frac{i^{-n+1}}{2n\pi} \int_{-1}^1 (-T_{n+1}(w) + T_{n-1}(w)) \frac{e^{iwt}}{\sqrt{1-w^2}} dw \\ &= \frac{i^{-n+1}}{n\pi} \int_{-1}^1 U_n(w) e^{iwt} dw , \end{aligned}$$

since

$$\begin{aligned} T_{n-1}(w) - T_{n+1}(w) &= \cos[(n-1)\arccos \theta] - \cos[(n+1)\arccos \theta] \\ &= 2\sin(n\arccos \theta)\sin(\arccos \theta) \\ &= 2U_n(w) \cdot U_1(w) \\ &= 2\sqrt{1-w^2} U_n(w) . \end{aligned}$$

Hence,

$$\frac{J_n(t)}{t} = \frac{2i^{1-n}}{n\pi} \int_0^1 U_n(w) \cos(wt) dw \quad (\text{A.7})$$

when n is an odd integer.

APPENDIX B. COLLECTION OF SOLUTIONS OF $\left[\frac{dw}{dz}\right]^2 = P(w)$

$$d < c < b < a$$

$P(w)$	region	$w(z)$	g	k^2
$(a-w)(b-w)(w-c)$	$[c, b]$	$c + (b-c) \operatorname{sn}^2(gz, k),$ $\frac{b-c}{a-c} \operatorname{sn}^2(gz, k)$	$\frac{\sqrt{a-c}}{2}$	$\frac{b-c}{a-c}$
$(a-w)(w-b)(w-c)$	$[b, a]$	$a - (a-b) \operatorname{sn}^2(gz, k),$ $\frac{a-b}{a-c} \operatorname{sn}^2(gz, k)$	$\frac{\sqrt{a-c}}{2}$	$\frac{a-b}{a-c}$
$(a-w)(b-w)(c-w)(w-d)$	$[d, c]$	$d + \frac{c-d}{a-c} \operatorname{sn}^2(gz, k),$ $\frac{c-d}{b-d} \operatorname{sn}^2(gz, k)$	$\frac{\sqrt{(a-c)(b-d)}}{2}$	$\frac{(a-b)(c-d)}{(a-c)(b-d)}$
$(a-w)(w-b)(w-c)(w-d)$	$[c, b]$	$c - \frac{b-c}{b-d} \operatorname{sn}^2(gz, k),$ $\frac{b-c}{a-c} \operatorname{sn}^2(gz, k)$	$\frac{\sqrt{(a-c)(b-d)}}{2}$	$\frac{(b-c)(a-d)}{(a-c)(b-d)}$
$(a-w)(w-b)(w-c)(w-d)$	$[b, a]$	$b - \frac{a-b}{a-c} \operatorname{sn}^2(gz, k),$ $\frac{a-b}{b-d} \operatorname{sn}^2(gz, k)$	$\frac{\sqrt{(a-c)(b-d)}}{2}$	$\frac{(a-b)(c-d)}{(a-c)(b-d)}$
$(a-w)(w-b)\{(w-c)^2 + d^2\}$	$[b, a]$	$\frac{aB + bA + (Ab - aB) \operatorname{cn}(gz, k)}{A + B + (A - B) \operatorname{cn}(gz, k)},$ $A^2 = (a-c)^2 + d^2,$ $B^2 = (b-c)^2 + d^2$	$\frac{\sqrt{AB}}{2}$	$\frac{(a-b)^2 - (A-B)^2}{4AB}$

APPENDIX C

ON THE TWO SOLUTIONS OF $\left(\frac{dw}{dz}\right)^2 = P(w)$

The differential equations which we are interested in is of the following form:

$$\left(\frac{dw}{dz}\right)^2 = P(w) \quad (C.1)$$

where $P(w)$ is a cubic or quartic polynomial.

We showed in Appendix B that the solutions of the above equation are expressed in terms of the Jacobian elliptic functions, sn , cn and dn . Corresponding to the fact that the circular functions sine and cosine are both the solutions of

$$\left(\frac{dw}{dz}\right)^2 = 1-w^2$$

with different initial conditions at $z=0$, there are also two solutions to (C.1) with different initial conditions at $z=0$. These two solutions can be matched by shifting one of them by a quarter period, as is the case for the circular functions:

$$\cos z = \sin\left(z + \frac{\pi}{2}\right).$$

For example,

$$\left(\frac{dw}{dz}\right)^2 = (a-w)(w-b)(w-c)$$

has two solutions,

$$w_1 = a - (a-b) \text{sn}^2\left(\frac{\sqrt{a-c}}{2} z, k\right), \quad k^2 = \frac{a-b}{a-c}$$

and

$$w_2 = \frac{b-c \frac{a-b}{a-c} \text{sn}^2\left(\frac{\sqrt{a-c}}{2} z, k\right)}{1 - \left(\frac{a-b}{a-c}\right) \text{sn}^2\left(\frac{\sqrt{a-c}}{2} z, k\right)}.$$

By using the following formula⁽⁴⁷⁾

$$\operatorname{sn}^2(x+K) = \frac{\operatorname{cn}^2(x)}{\operatorname{dn}^2(x)} = \frac{1-\operatorname{sn}^2(x)}{1-k^2\operatorname{sn}^2(x)},$$

we can show that

$$\begin{aligned} w_1\left(z + \frac{2K}{\sqrt{a-c}}, k\right) &= a - (a-b) \cdot \frac{1-\operatorname{sn}^2}{1 - \frac{a-b}{a-c}\operatorname{sn}^2} \\ &= \frac{a - \frac{a(a-b)}{a-c}\operatorname{sn}^2 - a + b + (a-b)\operatorname{sn}^2}{1 - \frac{a-b}{a-c}\operatorname{sn}^2} \\ &= \frac{b - \frac{(a-b)(a-a+c)}{a-c}\operatorname{sn}^2}{1 - \frac{a-b}{a-c}\operatorname{sn}^2} \\ &= \frac{b - c \cdot \frac{a-b}{a-c}\operatorname{sn}^2}{1 - \frac{a-b}{a-c}\operatorname{sn}^2} \equiv w_2(z, k). \end{aligned}$$

Hence we can choose one of the solutions to (C.1) to discuss the nature of the periodic solutions without losing generality.

APPENDIX D
COMPUTER PROGRAM

FILE: SUL/XXIV

```

      BEGIN
** THIS PROGRAM COMPUTES THE HEAT FLUX AND TEMPERATURE GRADIENT
** OF ONE DIMENSIONAL ANHARMONIC LATTICE WITH FORCE FUNCTION
**  $F = X + \text{ALPHA} X^2 + \text{RI} X^3$ 
** AND IMPACT TYPE HEAT RESERVOIRS AT BOTH ENDS.*
** WRITTEN 2/24/73 AND REVISED 3/25/73 K.MIURA
      FILE STATI(N(KIND=3,MAXRECSIZE=20,INTMODF=4,MYUSF=3);
      FILE LINE(KIND=7,MAXRECSIZE=22);
      FORMAT DIT
      FLF(X10,F9.2,X3,E10.3,X3,E10.3);
      FRF(X65,F9.2,X3,E10.3,X3,E10.3);
      F11(X1,I3,10(X2,R9.2));
      LABEL L4,L5;
      REAL ALPHU,ALI3,RI,RI4,R2,R6,HZSCL,H2,H4,HI3,HI5,ZMX;
      REAL K4,K5,K6,K7,K8,K9,H,I3,I6,I9,I192,H1192,HM23,H80;

      REAL AMP,WIDTH,SUM,TMP,RFLUX,LFLUX,TMH,YIP1,YI1,ZI1,H2I3;

      REAL ARRAY Y,4[0:51],TP,TQ[1:50,0:51];
      REAL ARRAY K1,K2,K3[1:51],KNT[1:50],LF,RF[1:300];
      INTEGER ARRAY XCO,YCO[1:100];
      INTEGER LCNTR,RCNTR,TW035;
      INTEGER I,J,K,L,M,JJ,KK,LL,L1,FLG,FLG2,FLG3;
      INTEGER X; %FOR RANDOM NUMBERS
      INTEGER N,TIME,STP,ISTART,ILAST,HI;

      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      REAL PROCEDURE RNDX;
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      BEGIN % DUE TO D.KNUTH
      X:=SECONDWORD(DINTEGER(3141592653 MUX X)+DINTEGER
      (2718281829)) MOD TW035;
      RNDX:=X/TW035;
      END; %RNDX %
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      REAL PROCEDURE MAXWELL(T); REAL T;
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      BEGIN
      %ONE DIMENSIONAL MAXWELL-HOLTZMANN DISTRIBUTION
      %
      REAL TMP;
      TMP:=-T*LN(1-RNDX);
      MAXWELL:=SQRT(TMP+TMP); %T IS ALWAYS ASSUMED TO BE POSITIVE
      END; % MAXWELL-HOLTZMANN %
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      PROCEDURE LSSU(A,IS,IL,INTL,ICPT,SLOP);
      VALUE IS,IL,INTL;
      INTEGER IS,IL,INTL;
      REAL ARRAY A[*];
      REAL ICPT,SLOP;
      XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      BEGIN
      REAL T1;
      INTEGER I,J;
      REAL SUMY,SUMZ,MAX,TEMP;
      SUMY:=SUMZ:=MAX:=TEMP:=0;

```

```

      FOR I:=IS STEP INTL UNTIL IL DO
      BEGIN
        J:=I/INTL;
        SUMY:=SUMY+I;
        TEMP:=TEMP+I*A[J];
        SUMZ:=SUMZ+A[J];
        MAX:=MAX+I*I;
      END;
      J:=(IL-IS)/INTL+1;
      T1:=J*MAX-SUMY**2;
      ICPT:=(SUMZ*MAX-SUMY*TEMP)/T1;      ***INTERCEPT
      SLOP:=(J*TEMP-SUMY*SUNZ)/T1;      **SLOPE
    EN) OF LEAST SQUARE FITTING;
***XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
PROCEDURE HAZELPLOT(XC0,YC0,N,MS);
VALUE N,MS;
INTEGER N,MS;
INTEGER ARRAY XC0,YC0[*];
***XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
BEGIN
  FORMAT OUT FO(4"A11UA11DA11FA11040200") .
  F1(F5.2 " ">">,12(".....").".....<">,4"00").
  F2(X5,"=",X64,"=">.4"00").
  F3(X5,"00",13("''''"),4"00").
  F4(X3,13(13*X2)*4"A11200");
  OWN INTEGER SCALEFLG; INTEGER I;ARRAY X[0:0];
  POINTER P,Q;
  VALUE ARRAY ASCII
  (4"0401020372D2E2F160525080C0D0E0F101112133C3D32"
  4"2618193F21C1D1E1f"" ""'()*+,-./0123456789"
  "1;<=>?@ACUFGHIJKL~NNPQRSTUVWXYZ[">4"E0""")~"
  4"4B/98182D3D485D6D/H8889919293949596979899A2A3A4A5"
  4"A6A7A8A9CU6AD0A10/") ;
  X
  &
  P:=POINTER(X)+2;
  Q:=POINTER(ASCII);
  REPLACE POINTER(X[0]) BY 4"A111" FOR 2." " FOR 2.
    4"4E00" FOR 2;
  WRITE(STATION,F0);
  IF SCALEFLG=0 THEN
    BEGIN
      SCALEFLG:=1;
      WRITE(STATION,<4"A11CA11CA119A11900">);
      FOR I:=0 STEP 1 UNTIL 24 DO BEGIN
        IF I MOD 5=0 THEN
          WRITE(STATION,F1,(15-I)/H2SCL)
            ELSE WRITE(STATION,F2); END;
      WRITE(STATION,F3);
      WRITE(STATION,F4,FOR I:=0 STEP 5 UNTIL 60 DO I);
      WRITE(STATION,<4"A11FA11FU0">);
      END;
      WRITE(STATION,<4"A11200">);
      WRITE(STATION,<"TIME=">.15.X3,"ENRGY=">.R11.5.X3,"ALPHA=">.E11.4>
        .MS.SUM.ALPHU);
      FOR I:=1 STEP 1 UNTIL N DO
        BEGIN
          YC0[I]:=YC0[I]+15;
          REPLACE P BY Q+XC0[I] FOR 1.Q+YC0[I] FOR 1;

```

```

WRITE(STATION,1,X[*]);                                00012100
END;                                                    00012200
WRITE(STATION,<4"A112A11900">);                        00012300
END OF HAZELTIME;                                     00012400
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 00012500
PROCEDURE KINETICTEMP(N,X,TIME,N1);                   00012600
  VALUE N,TIME,N1;                                     00012700
  INTEGER N,TIME,N1;                                   00012800
  REAL ARRAY X[*];                                     00012900
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 00013000
BEGIN                                                  00013100
  FORMAT OUT                                           00013200
  F51 (X5," KINETIC TEMPERATURE AT",                00013300
      " TIME =",I4),                                  00013400
  F52(X20,"I", 5(9("",""),"I"),),                  00013500
  F56(X1,E13.6,X2,I2,X2,"0"),,                      00013600
  F54(X1,E13.6,X2,I2,X2,"0",*("X"),),               00013700
  F57(X20,"0",X8,".2",X8,".4",X8,".6",X8,".8",X7,   00013800
      "1.0");                                          00013900
  INTEGER I,J,K;                                       00014000
  REAL T1,T2, TAX,TEMP;                               00014100
  REAL ARRAY FOURIER[1:N];                            00014200
  WRITE(LINE[SKIP 1]);                                00014300
  TMH:=TIME*HI;                                        00014400
  TAX:=AMP+AMP;                                        00014500
  FOR I:=1 STEP 1 UNTIL N DO                          00014600
    TAX:=MAX((FOURIER[I]:=X[I]/TMH),TAX);             00014700
    WRITE(LINE ,F51,TIME);                            00014800
    WRITE(LINE ,F57);                                  00014900
    WRITE(LINE ,F52);                                  00015000
    T1:=100/TAX;                                       00015100
    FOR I:=1 STEP 1 UNTIL N1 DO                       00015200
      BEGIN                                           00015300
        K:=T1*(TEMP:=FOURIER[I]);                   00015400
        IF K NEQ 0 THEN                              00015500
          WRITE(LINE ,F54,TEMP,I,K) ELSE             00015600
          WRITE(LINE ,F56,TEMP,I);                   00015700
        END;                                           00015800
        WRITE(LINE ,F52);                             00015900
        WRITE(LINE ,F57);                             00016000
        WRITE(LINE,</"ACCUM.LFLUX=" ,R12.5,X5,"ACCUM. RFLUX=" 00016100
            ,R12.5/> ,LFLUX,RFLUX);                  00016200
        LSSQ(FOURIER,1,N,1,T1,T2);                  00016300
        WRITE(LINE,<"SLOPE=" ,E12.5,X3,"LEFT LSQ TMP=" , 00016400
            E12.5,X3,"RIGHT LSQ TMP=" ,E12.5>,T2,T1+T2, 00016500
            T1+N*T2);                                  00016600
        WRITE(LINE,</X10,"LEFT COL=" ,I6,X35,"RIGHT COL=" ,I6>, 00016700
            LCNTR,RCNTR);                             00016800
        WRITE(STATION,F51,TIME);                     00016900
        WRITE(STATION,<"ACCUM.LFLUX=" ,R12.5,X5,"ACCUM. RFLUX=" 00017000
            ,R12.5/>,"LEFT COL=" ,I6,X5,"RIGHT COL=" ,I6,<"/, 00017100
            "SLOPE " ,E12.5,<"/,"T25 " ,E12.5>,LFLUX*,5. 00017200
            RFLUX*.5,LCNTR,RCNTR,T2,FOURIER[25]);    00017300
      END; %%%KINETIC TEMPERATURE %%%                00017400
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 00017500
PROCEDURE POLYGRAPH(P,N,W,SCALE);                   00017600
  VALUE P,N,SCALE;                                    00017700
  INTEGER P,N,SCALE;                                  00017800
  REAL ARRAY W[*,*];                                  00017900
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 00018000
COMMENT THIS PROCEDURE DISPLAYS 10 GRAPHS USING A LINE 00018100

```

```

PRINT. THEY SHOULD NOT OVERLAP. W CONTAINS THE
DATA. N IS THE NUMBER OF GRAPHS. P IS THE
STARTING POINT OF ABSCISSA.;
00018200
00018300
00018400
00018500
00018600
00018700
00018800
00018900
00019000
00019100
00019200
00019300
00019400
00019500
00019600
00019700
00019800
00019900
00020000
BEGIN
FORMAT OUT F0(X4,12(I3,X7)),
F1(X6,11("V",9("n")),nVn),
F2(X1,I4,X1,12(X*,n*n));
F3(X6,11("X",9("n")),nXn),
FFF(I3,10(F12,8),I4),
F4(I3,10(F12,10),I4),
F2(X1,I4,X1,X*,n,n,2(X*,n*n,X*,n*n,X*,n,X*,
n0",X*,n5n));
00020100
00020200
00020300
00020400
00020500
00020600
00020700
00020800
00020900
00021000
00021100
00021200
00021300
00021400
00021500
00021600
00021700
00021800
00021900
00022000
00022100
00022200
00022300
00022310
00022320
00022400
00022500
00022600
00022700
00022800
00022900
00023000
00023100
00023200
00023300
00023400
00023500
00023600
00023700
00023800
00023900
00024000
00024100
INTEGER I,J,K,TMP,L;
INTEGER ARRAY Y(1:10);
WRITE(LINE,<"V1",x12,"v2 ",x11,"QUAD",x10,"CURR",x10,"SCALE",
x10,"STEPSIZE">);
WRITE(LINE,<6(R11.4,X3)/>,AMP,WIDTH,ALPHA,RI,SCALE,H);
FOR I:=0 STEP 1 UNTIL N DIV 10 -1 DO
BEGIN
WRITE(LINE,F0,FOR J:=0 STEP 1 UNTIL 10 DO
P+I+10+J);
WRITE(LINE,F1);
FOR J:=1 STEP 1 UNTIL N DO
BEGIN
FOR K:=1 STEP 1 UNTIL 10 DO
IF TMP:=I+10+K LEQ N THEN
Y[K]:=W[TMP,J]*SCALE;
WRITE(LINE,F2,J,0,9+Y[1],9+Y[2]-Y[1],
9+Y[3]-Y[2],9+Y[4]-Y[3],9+Y[5]-Y[4],
9+Y[6]-Y[5],9+Y[7]-Y[6],9+Y[8]-Y[7],
9+Y[9]-Y[8],9+Y[10]-Y[9]);
END;
WRITE(LINE,F3);
WRITE(LINE(SKIP 1),F0,FOR J:=0 STEP 1 UNTIL 11
DO (P+J+10+J));
FOR J:=0 STEP 50 UNTIL N DIV 50 -1 DO
BEGIN
WRITE(LINE,<X3,10(I5,X7)/>,FOR L:=1 STEP 1
UNTIL 10 DO (P+I+10+L));
FOR L:=1 STEP 1 UNTIL 50 DO
WRITE(LINE,FFF,J+L,FOR K:=1 STEP 1 UNTIL
10 DO W[K+I+10,J+L],J+L);
WRITE(LINE,F4,J+51,FOR K:=1 STEP 1 UNTIL
10 DO W[K+I+10,J+51],J+51);
WRITE(LINE(SKIP 1));
END;
END;
66PRINTLINE %
REAL PROCEDURE V(X); VALUE X; REAL X;
BEGIN
V:=X*(1+X*(+ALPHA)+RI*X));
END;
PUT:=X*X*(.5+X*(ALI3+RI4*X));
END;

```

```

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX00024200
PROCEDURE NYS4(N,Y,Z);00024300
VALUE N;00024400
INTEGER N;00024500
REAL ARRAY Y,L[0];00024600
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX00024700
*00024800
* THIS PROCEDURE PERFORMS ONE STEP OF RUNGE-KUTTA00024900
* METHOD(NYSTROM'S FORMULA). THE EQUATION IS00025000
*  $(U+2)Y/DX+2=DIFFUN(Y)$ 00025100
* WITH INITIAL VALUES  $Y$ -AND  $DY/DX=Z$ .00025200
*  $Y$  IS A VECTOR WHOSE ELEMENTS ARE00025300
*  $Y[0],Y[1],\dots,Y[N]$ .00025400
*  $H$  IS STEP SIZE,I.E.  $Y$  AT  $X+H$  IS EVALUATED00025500
* FROM  $Y$  AT  $X$ .00025600
* BOTH ENDS ARE FREE.00025700
* REVISED ON MAY 24 1972 K.MIURA00025800
* REVISED ON MAY 29 K.MIURA00025900
*00026000
*00026100
BEGIN00026200
INTEGER I;00026300
K5:=K7:=K9:=0;00026400
YIP1:=Y[1];00026500
FOR I:=1 STEP 1 UNTIL N DO00026600
BEGIN00026700
K4:=K1[I]:=-K9+(K9:=V(-(YI1:=YIP1)+(YIP1:=Y[I00026800
+1])));00026900
K6:=K5; *K6=Y1[I-1]00027000
K5:=YI1+.4*((ZI1:=Z[I])+.2*K4*H)*H/*1 ST IT00027100
K2[I]:=V(K5-K6); **K2 TEMPORARY USE FOR VT00027200
K8:=K7; *Y2[I-1]00027300
K7:=YI1+H2*(ZI1/3+H*K4/9); *2ND ITERATION]00027400
K3[I]:=V(K7-K8);00027500
END;00027600
K5:=0;00027700
K2[1]:=K3[1]:=K2[N+1]:=K3[N+1]:=0;00027800
FOR I:=1 STEP 1 UNTIL N DO00027900
BEGIN00028000
YI1:=00028100
K2[I]:=K2[I+1]-K2[I];00028200
K3[I]:=K3[I+1]-K3[I];00028300
K6:=K5; *Y30028400
K5:=Y[I]+.80*(Z[I]+.20*((ZI1:=K1[I])+YI1)+H)*H;00028500
Z[I]:=**H*H23*ZI1/192;00028600
K1[I]:=V(K5-K6); *K1 TEMPORARILY USED FOR V00028700
END;00028800
K1[1]:=K1[N+1]:=0;00028900
FOR I:=1 STEP 1 UNTIL N DO00029000
BEGIN00029100
K4:=K1[I+1]-K1[I];00029200
Y[I]:=**H*(Z[I]+H*(75*(YI1:=K2[I])00029300
-(K6:=27*K3[I])+25*K4)/192);00029400
Z[I]:=**H*(125*(YI1+K4)-(K6+K6+K6))/192;00029500
END;00029600
Y[N+1]:=Y[N];00029700
END; *NYSTROM FREE BOUNDARY REVISED00029800
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX00029900
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX00030000
WRITE(STATION,<X10,"TYPE IN PARAMETERS IN THE FOLLOWING"00030100
00030200
00030300

```

```

      . " ORDER"//
      \ " # OF ATOMS" / "LEFT TEMPERATURE" / "RIGHT TEMPERATURE" /
      "QUADRATIC COEFF." / "CUBIC COEFF." / "TIME LIMIT" / "INITIAL CONDITION"
/" IF RANDOM PUT 1 AND SPECIFY YIN AND ZIN . "
/" IF TRANSMISSION PROPERTIS ARE TO BE STUDIED , PUT 0" /
" IN WHICH CASE LEFT TEMP AND RIGHT TEMP ARE INITIAL VEL"
/" YIN" / " ZIN" / "PRINT Y&Z(PUT 1 IF SO AND SPECIFY SCALINGS)"
/" SCALE Y" / " SCALE Z" / "TIME INCREMENT" / "PRINT TEMPERATURE( IF SO"
" SPECIFY THE INTERVAL AT WHICH YOU WANT THE GRAPH"
/" BOUNDARY CROSS CHECKING" / "HAZELTIME INTERVAL(0 IF NO NEED)"
/"HAZELTIME SCALING(0 IF NOT NEEDED"//>);

READ(STATION,/,N,AMP,WIDTH,ALPHU,RI,TIME,STP,TMP,SUM,FLG,ISTART,
ILAST,H,FLG3,L1,FLG2,HZSCL);
WRITE(STATION,< //x10."THANK YOU ">);
WRITE(LINE ,<10R10.3/7R10.3>*N*AMP,
      WIDTH,TIME,STP,ALPHU,RI,FLG,ISTART,ILAST,
      H,FLG3,L1,SUM,TMP);

*****CONSTANTS *****
      ALI3:=ALPHU/3;
      RI4:=RI/4;
      HM23:=H*23;

      HI:=1/H; ***** INVERSE

      H2:=H*2;

      HI5:=H*.2;
      TWI35:=2*.35;
*****INITIAL CONDITIONS *****
FOR I:=1 STEP 1 UNTIL 1000 DO HI3:=RNDX; *****IDLING OF
      ZMX:=(AMP+WIDTH)*SUM;
      IF STP EQL 1 THEN ***** THERMAL SITUATION
      FOR J:=1 STEP 1 UNTIL N DO
      BEGIN
      Y[I]:=TMP*(RNDX-.5);

      Z[I]:=IF RNDX GEQ .5 THEN MAXWELL(ZMX)
      ELSE -MAXWELL(ZMX);
      END)
      ELSE ***** TRANSMISSION PROPERTY

      BEGIN
      Z[1]:=AMP;

      Z[N]:=-WIDTH;
      END);
      Y[N+1]:=Y[N];
      KI:=0;
      FOR II:=1 STEP 1 UNTIL N DO
      XCU[II]:=I+6;
*****
L4: IF K < TIME THEN

      BEGIN

```

```

      KK:=K/50+1;                                00036400
COMMENT                                           00036500
      WRITE(LINE[SKIP 1]);                          00036600
COMMENT                                           00036700
      WRITE(LINE,<X20,"COLLISIONS BETWEEN TIME=",I4,
        " AND TIME=",I4, "//X4,"(LEFT)",X4,"TIME",X5,
        "VELOCITY",X25,"(RIGHT)",X6,"TIME",X5,"VELOCITY"/
        X23,"(FROM)",X10,"(TO)",X35,"(FROM)",X10,"(TO)"/>
        ,K,K+50);                                00037000
      FOR J:=1 STEP 1 UNTIL 50 DO                 00037100
        BEGIN                                     00037200
          FOR JJ:=1 STEP 1 UNTIL HI DO             00037300
            BEGIN                                 00037400
              IF JJ MOD L1 EQL 0 THEN              00037500
                BEGIN                             00037600
                  IF Y[1]+H*(ZMX:=Z[1])<-.0001 THEN 00037700
                    BEGIN                         00037800
                      LCNTR:=LCNTR+1;             00037900
                      ZI1:=                        00038000
                      Z[1]:=MAXWELL(AMP)           00038100
COMMENT                                           00038200
                      WRITE(LINE,FLF,K+J+H,ZMX,ZI1); 00038300
                      LFLUX:=LFLUX+(ZI1 +ZMX)*(ZI1 -ZMX); 00038400
                      END;                         00038500
                      IF Y[N]+H*(ZMX:=Z[N])>.0001 THEN 00038600
                        BEGIN                     00038700
                          RCNTR:=RCNTR+1;         00038800
                          ZI1:=                    00038900
                          Z[N]:=-MAXWELL(WDTH);    00039000
                          RFLUX:=RFLUX-(ZI1 +ZMX)*(ZI1 -ZMX); 00039100
COMMENT                                           00039200
                          WRITE(LINE,FRF,K+J+H,ZMX,ZI1); 00039300
                          END;                     00039400
                        EN) OF COLLISIONS WITH HEAT RESERVOIR; 00039500
                      NYS4(N ,Y,Z);                00039600
                      FOR I:=1 STEP 1 UNTIL N DO    00039700
                        KNTp[I]:=**+Z[I]**2;        00039800
                      END OF JJ LOOP;              00039900
                      IF FLG EQL 1 THEN *PRINT Y AND Z 00040000
                    BEGIN                           00040100
                      Y[N+1]:=Y[N]; SUM:=0;         00040200
                      ZMX:=0;                       00040300
                      FOR I:=1 STEP 1 UNTIL N DO    00040400
                        BEGIN                       00040500
                          ZI1:=TQ[J,I]:=Z[I];      00040600
                          SUM:=**+.5*(ZI1+ZI1+ZMX  00040700
                            +(ZMX:=POT(TP[J,I]):=  00040800
                              Y[I+1]-Y[I])));      00040900
                          END;                      00041000
                        TP[J,N]:=Y[1];              00041100
                        TP[J,N+1]:=Y[N];            00041200
                        TQ[J,N+1]:=SUM; % TOTAL ENERGY 00041300
                      END OF SAVING DATA FOR PRINTING; 00041400
                      IF FLG2 NEQ 0 THEN IF J MOD FLG2 EQL 0 THEN 00041500
                        BEGIN % HAZELTIME            00041600
                          FOR I:=1 STEP 1 UNTIL N DO 00041700
                            YCO[I]:=Z[I]+HZSCL;    00041800
                            HAZELPLUT(XCO,YCO,N,K+J); 00041900
                          END HAZELTIME;             00042000
                        END OF J LOOP;               00042100
                      END OF J LOOP;                 00042200
                    END OF J LOOP;                   00042300
                  END OF JJ LOOP;                   00042400
                END OF JJ LOOP;                     00042500
              END OF JJ LOOP;                       00042600
            END OF JJ LOOP;                         00042700
          END OF JJ LOOP;                           00042800
        END OF JJ LOOP;                             00042900
      END OF JJ LOOP;                               00043000
    
```

```

LF(KK):=LFLUX;
RF(KK):=RFLUX;
IF FLG3 NEQ 0 THEN IF K MOD FLG3 EQL 0 THEN
    KINETICTEMP(N,KNTF,K+50,N);
    IF FLG EQL 1 THEN *PRINT Y AND Z
    BEGIN
        POLYGRAPH(K,N,TP,ISTART); * COORDINATE
        POLYGRAPH(K,N,TQ,ILAST); **VELOCITY
    END;
IF (J:=K+50) MOD 1000 EQL 0 THEN
    BEGIN
        WRITE(LINE,SKIP 1);
        WRITE(LINE,<X10,"FLUX LEAST SQUARE FITTING AT ",I5/
            X5,"LEFT",X25,"RIGHT"/>,J);
        FOR L:=100 STEP 100 UNTIL J-500 DO
            BEGIN
                LSSQ(LF,L,J,50,SUM,ZMX);
                LSSQ(RF,L,J,50,SUM,ZI1);
                WRITE(LINE,<2(X5,I5,X2,E11.4)>,.L,ZMX*,5,
                    L,ZI1*,5);
            END IF FLUX LEAST LINEAR FITTING;
        WRITE(STATION,</"MORE? IF SO, TYPE 1"/>);
        READ(STATION,/,M);
        IF M NEQ 1 THEN
            GO TO L5;
        END; ***K MOD 1000
        K:=K+50;
        GO TO L4;
    END; **** IF K LOOP(50 SEC);
L5:
    END.

```

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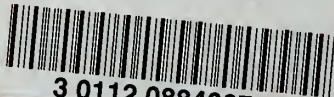
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